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(54) Title: MODIFIED DEACETOXYCEPHALOSPORIN C SYNTHASE (DAOCS) AND X-RAY STRUCTURE

(57) Abstract

Three-dimensional crystal structure(s) of deacetoxycephalosporin C synthase (DAOCS) are described. The X-ray co-ordinates provide precise 3-dimensional information of amino acids within the structure of DAOCS. Some of these are in complexes with iron and/or substrates. Information from the structures is used to modify enzymes of the cephalosporin biosynthesis pathway including DAOCS, deacetylcephalosporin C synthase DAOC/DACS, such that they accept unnatural substrates (e.g. penicillins G, V) in order to improve the production of beta-lactam antibiotics. The structures may be used to predict the structures of other 2-oxoglutarate dependent enzymes, thereby allowing the design of inhibitors, and new catalysts for the production of e.g. oxidised amino acids/peptides. Specific modifications of amino acid residues are proposed and exemplified.

U.S. Patent Application No. 10/719,237 Attorney Docket No. 6653-020-999 Reference AN

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MODIFIED DEACETOXYCEPHALOSPORIN C SYNTHASE (DAOCS) AND X-RAY STRUCTURE

- Penicillin and cephalosporin antibiotics are produced either directly by fermentation or by modification of fermentation derived materials containing a beta-lactam ring. The biosynthetic pathway to the penicillins and cephalosporins has been extensively studied and reviewed (J. E. Baldwin and C. J. Schofield, in 'The Chemistry of β-lactams (Ed. M. I. Page), Chapter 1, Blackie, London 1992; Ingolia and Queener, Med. Res. Rev., 1989, 9, 245-264; Aharonowitz, Cohen and Martin, Ann. Rev. Microbiol., 1992, 46, 461-495; Schofield, Bycroft, Baldwin, Hadju, Roach, Current Opinion in Structural Biology, 1997, 7, 857-864) and includes the following steps (Figure 1):
- 1. Conversion of the tripeptide: <u>L</u>-δ-α-aminoadipoyl-<u>L</u>-cysteinyl-<u>D</u>-valine (ACV) to isopenicillin N in a step catalysed by isopenicillin N synthase (IPNS). This step is common to both penicillin and cephalosporin biosynthesis.
 - 2. In some organisms (e.g. Penicillium chrysogenum and Aspergillus nidulans) isopenicillin N is converted by exchange of its <u>L</u>-δ-α-aminoadipoyl side chain to penicillins with other side chains, which are normally more hydrophobic than the side chain of isopenicillin N. This conversion is catalysed by an amidohydrolase/ acyltransferase enzyme. Examples of penicillins produced by this biosynthetic process include penicillin G (which has a phenylacetyl side chain) and penicillin V (which has a phenoxyacetyl side chain). These hydrophobic penicillins may be commercially produced via fermentation under the appropriate conditions.
 - 3. In other organisms (e.g. *Streptomyces clavuligerus* and *Cephalosporium acremonium*) isopenicillin N is epimerised to penicillin N. This reaction is catalysed by an epimerase enzyme.

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- 4. In some organisms (e.g. S. clavuligerus and C. acremonium) penicillin N is converted to DAOC. This reaction is catalysed by deacetoxycephalosporin C synthase (DAOCS) in some organisms (e.g. Streptomyces clavuligerus) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others (e.g. C. acremonium).
- 5. In some organisms (e.g. *S. clavuligerus* and *C. acremonium*) DAOC is converted to deacetylcephalosporin C (DAC). This reaction is catalysed by deacetylcephalosporin C synthase (DACS) in some organisms (e.g. *S. clavuligerus*) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others (e.g. *C. acremonium*).

Further biosynthetic steps to give other cephalosporin derivatives may also occur, e.g. in *C. acremonium* DAC may be converted to cephalosporin C and in *Streptomyces spp*. DAC may be converted to cephamycin C. The genes encoding for each of the enzymes catalysing steps 1-6 above have been identified and sequenced.

Fermented penicillins, cephalosporins and their biosynthetic intermediates are useful as antibiotics or as intermediates in the production of antibiotics. Penicillins with hydrophobic side chains may be used for the preparation of cephalosporins or intermediates used in the preparation of cephalosporins, e.g. penicillins (including penicillin G and penicillin V) may be used to prepare C-3 exomethylene cephams which may be used as intermediates in the preparation of the commercial antibiotics, e.g. Cefachlor.

The enzymes IPNS, DAOCS, DACS and DAOC/DACS are

members of an extended family of Fe(II) utilising oxidase and oxygenase
enzymes. Most of this family (including DAOCS, DACS and DAOC/DACS)
utilise a 2-oxo acid (normally 2-oxoglutarate) as a cosubstrate in addition to
dioxygen and the 'prime' substrate (e.g. penicillin N in the case of DAOCS).
Since IPNS, does not use 2-oxoglutarate, it has a substantially different
mechanism to the 2-oxoglutarate dependent oxygenases, and this gives

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rise to a significantly different active site.

The Invention

This invention is based on the determination of the three dimensional crystal structure of DAOCS and the information and developments which come from it. The X-ray co-ordinates provide very detailed 3-dimensional information on the relationships between amino acid residues in the structure of DAOCS and on the binding modes of the Fe-cofactor and the substrates to DAOCS. The structure allows the modification of DAOCS and related enzymes of penicillin and cephalosporin biosynthesis (including DACS and DAOC/DACS) in order to alter their substrate and product selectivities. Since the DAOCS structures are the first from the family of 2-oxoglutarate dependent dioxygenases they also allow for the design of new inhibitors of this family of enzymes.

Previously partial overviews of the structures of IPNS complexed to manganese and IPNS complexed to iron and ACV were reported (Roach et al., Nature, 1995, 375, 700-704; Roach et al., Nature, 1997, 387, 827). The structures, as defined by their X-ray co-ordinates, of IPNS complexed to manganese and in complexes with iron, ACV and/or substrate analogues have been reported in Baldwin, Hajdu, Roach, Hensgens, Clifton, GB 9621486.1- (Oxygenase Enzymes and Method).

Procedures have been developed for the production of 7-aminodeacetoxycephaosporin C (7-ADCA) in which recombinant *P. chrysogenum* strains into which the DAOCS gene has been introduced are used for the production of cephalosporins. In particular if adipic acid is added to these recombinant strains adipoyl-6-APA is produced, which is converted by DAOCS into adipoyl-7-ADCA from which the adipoyl side chain can be removed (EPA-A-0532341, Shibata *et al.*, Bioorg. Med. Chem. Letts, 1996, 6, 1579-1584).

The IPNS gene sequence (and therefore the amino acid

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sequence) is related but significantly different to those of DAOCS, DACS, DAOC/DACS. It is likely that gross elements of the fold (i.e. significant elements within the 3-dimensional structure) of these enzymes will be conserved but that the active site architecture will be very significantly different. Structural elements conserved are likely to include the beta-barrel 'jelly roll' core and certain alpha-helices (including alpha helix-10, as defined in Roach *et al.*, Nature, 1995, 375, 700-704). The degree of similarity is insufficient to define the precise structure of DAOCS, DACS, or DAOC/DACS from the IPNS structures. To date no models of DAOCS, DACS, or DAOC/DACS based on the IPNS structure have been reported. Nor have any detailed studies on substrate binding of these enzymes been reported. One report (WO 97/20053) claims the use of products resulting from modification of certain residues in DAOCS for the improved conversion of penicillin G to phenyl acetyl (G)-7-aminocephalosporanic acid.

The three-dimensional structure of DAOCS is defined by the X-ray co-ordinates set out below (Structure A).

Also set out below is a high resolution crystal structure of a complex of prokaryotic DAOCS from *S. clavuligerus* with Fe(II) and 2-oxoglutarate (Structure B).

In part the present invention relates to the use of the structures of DAOCS in order to make modifications to it or DACS or DAOC/DACS in order that the modified enzymes catalyse the conversion of unnatural penicillins (e.g. penicillin G and penicillin V) to cephalosporins more efficiently than the wild-type enzyme. Further aspects of the invention relate to the use of the DAOCS structure in order to produce unnatural products in micro-organisms. Such products include exomethylene cephalosporins, with or without alpha-aminoadipoyl or hydrophobic side chain (e.g. phenylacetyl or phenoxyacetyl). Thus one aspect of this invention refers to the use of the structure of DAOCS for modifying DAOCS



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(or the closely related enzymes DACS or DAOC/DACS) in order to:

- (i) permit the enzyme to accept (or accept more efficiently) unnatural penicillin substrates for the preparation of new or commercially valuable antibacterial materials.
- (ii) enable the modified enzyme to produce unnatural (e.g. exomethylene cephams) or optimise the production of minor products (e.g. 3-β-hydroxycephams) for use as antibacterials or as intermediates in the preparation of antibacterials or commercially valuable compounds.

In another aspect this invention provides modified enzymes that result from application of the aforementioned techniques. These are enzymes having significant (as defined below) sequence and thus structural similarity with DAOCS. Thus, structures of these enzymes may be predicted on the basis of the DAOCS structures. Preferably there will be sequence similarity/identity between most of the modified enzyme and a major part of DAOCS. Previous sequence comparisons (Roach et al., Nature, 1995, 375, 700), using pairwise comparisons of the sequences followed by single linkage cluster analysis show that IPNS, DAOCS, DACS and DAOC/DACS cluster with standard deviations scores of >5.0 (Barton and Sternberg, J. Mol. Biol., 1987, 198, 327). Scores over 5.0 and preferably over 6.0 indicate that the sequence alignments will be correct within all or most of the protein secondary structural elements (Barton, Methods in Enzymol., 1990, 183, 403); thus they have significantly similar sequences and hence structures. Note there are other criteria which may be used to ascertain significant sequence similarity for example % identity or % similarity of amino acids possessing side chains with similar physicochemical properties (Barton and Sternberg, J. Mol. Biol., 1987, 198, 327). Thus, on the basis of sequence comparisons it is possible to predict the structure of one enzyme (e.g. DACS or DAOC/DACS) from another closely related enzyme (e.g. DAOCS). Further, it is recognised that although two enzymes may have structures in which secondary structural elements are

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largely or wholly conserved, differences in the structures of the two enzymes may result from the side chains of the amino acids forming the secondary structural elements. The effect of these differences, which alter the substrate/product selectivities of the compared enzymes, is predictable once the three-dimensional structure of one of the enzymes is known.

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In another aspect the invention provides an enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the side chain binding site of penicillin N or DAOC is modified and at at least one of the following sites at least one amino acid residue is changed to another amino acid residue or is deleted: Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

Modifications of this kind will permit the expansion of penicillin V or penicillin G to the corresponding cephalosporins. To achieve this it is desirable to increase the kcat/Km for the mutant as compared to the wild type DAOCS. Kinetic results indicate that apparent kcat values for penicillin N and penicillin G are similar but that Km is much higher for penicillin G. Thus based on these analysis, a decrease in the binding constant of DAOCS for penicillin G should make it possible to increase kcat/Km for penicillin G.

The side chain binding pocket of DAOCS is made of residues from different parts of the peptide chain, so it is likely that more than one residue will have to be altered to make a better penicillin G/V expander. Nevertheless some residues are more important than others. Examination of the interactions between the last few C-terminal residues (Thr-308 to Ala-311) of one DAOCS molecule and the active site of another in the crystal structure, suggests a binding mode for the penicillin nucleus which

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is shown in Figure 2 of the accompanying drawings. The penam C-3 carboxylate group probably occupies an analogous position to that of Ala-311 from a symmetry related molecule in the active site, forming electrostatic interactions with Arg-162 and Arg-160. The side chain of Arg-160 may also form a hydrogen bonding interaction with the β -lactam carbonyl.

It needs to be borne in mind that protein specificity is generally controlled by more than one amino acid. To alter the specificity of a protein in a major way is likely to require more than one of the mutational changes suggested below, although each of the mutations will contribute. With this in mind, preferred residues to modify for the expansion of a penicillin are as follows:

- a) Arg-266. This residue binds with the α -aminoadipate side chain of the natural substrate and should be changed to a residue of more hydrophobic character, e.g. Phe, Ala, Val, Leu, Ile.
- b) Thr-72. This should be changed to a hydrophobic residue e.g. Val, Leu, Ile, Phe, Ala, to help bind the hydrophobic side chain of penicillin G. It should be effective in combination with other mutants.
- c) Arg-74 may be usefully changed to a neutral or hydrophobic residue (Phe, Tyr, Val, Leu, Ile, Ala). Modification of Arg-75 may be necessary in addition because it forms a hydrogen-bonding network with Arg-74.
 - d) Glu-156. This residue binds with the α -aminoadipate side chain. It should be changed to one of Ala, Val, Leu, Ile, Phe, Tyr, Trp, Asn, Gln, Ser.
- e) The side chains of Leu-158, Asn-301 and Tyr-302 form part of the binding pocket for the penicillin side chain and can be usefully modified to more hydrophobic character.
 - f) Asn-304. This residue binds the amide linking the side chain to the penam nucleus. Modification is effected to expand penicillins with shortened or no side chains (e.g. to Asp or Glu for 6-Apa).

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Note that other changes may be used to construct part or all of a side chain binding pocket via hydrogen bonding or other interactions.

The insertion or deletion of residues into the DAOCS sequence may also be of use in constructing a hydrophobic binding pocket for the penicillin side chain. Insertion of hydrophobic residues into the C-terminal region (residue 300-311 and in particular 301-303) may assist in the construction of a hydrophobic binding pocket for penicillin side chains.

In another aspect the invention provides an enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the penicillin/cephalosporin binding site of penicillin N or DAOC is modified and at at least one of the following amino acid residues is changed or deleted: Ile88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Asn304, Ile305, Arg306, Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

Further discussion of this aspect may be found in Nature Volume 394, pages 805-809 published on 20 August 1998 and incorporated by reference herein.

Another aspect of the invention refers to the use of the structure of DAOCS in order to modify its active site (or that of a structurally related 2-oxoglutarate dependent dioxygenase) in order that the modified enzyme accepts non beta lactam substrates in order to produce oxidised compounds of value. Oxidised amino acids (e.g. 4-hydroxyprolines, hydroxylysines, hydroxyaspartic acids and others) are useful as synthetic intermediates in the production of valuable materials. Using the structure of DAOCS specific residues can be targeted for modification in order that the modified enzyme can be used to produce oxidised amino acids or peptides. The process may include modification of the following residues:

Arg74, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304, Ile88, Arg162, Phe164, Met180, Thr190, Ile192, Pro241, Val245, Val262, Ile305, Arg306, Arg307.

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Another aspect of the invention refers to the use of the DAOCS structure for the design of selective inhibitors of 2-oxoglutarate dependent dioxygenases. The 2-oxoglutarate dependent dioxygenase prolyl 4-hydroxylase has been the target of inhibition in order to provide a therapeutic treatment for fibrotic diseases (e.g. liver cirrhosis, arthritis). However, no inhibitors are in clinical use, probably because it is difficult to achieve selective inhibition of the target enzyme for inhibition over other enzymes (including 2-oxoglutarate dependent enzymes). The structure of DAOCS provides a template for the design of inhibitors of 2-oxoglutarate dependent dioxygenases.

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Set out below are two high resolution crystal structures for DAOCS from S. clavuligerus: the structure of the iron-free apoenzyme (Structure A) and the structure of the complex with Fe(II) and 2-oxoglutarate (Structure B). The results imply a mechanism by which the enzyme-Fe(II) complex reacts with 2-oxoglutarate and dioxygen to give the reactive ferryl species, a process common to many non-haem oxygenases. Other notable 2-oxoacid-dependent ferrous enzymes are prolyl hydroxylase, involved in collagen biosynthesis, gibberellin 3β-hydroxylase, a mutation of which influences stem length in plants, and clavaminic acid synthase, involved in the biosynthesis of the β -lactamase inhibitor, clavulanic acid. Within the family of 2-oxoacid-dependent enzymes, DAOCS belongs to a sub-family, the members of which show sequence similarity with IPNS and 1-aminocyclopropane-1-carboxylate oxidase (the ethylene forming enzyme), enzymes that do not use a 2-oxoacid in catalysis.

The iron-free form of DAOCS crystallises in space group R3

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as a crystallographic trimer. The main chain of the protein folds into a conserved jelly roll core with flanking helices.

Co-ordinates and structure factors have been deposited with the Protein Data Bank (entries 1rxg, and r1rxgsf for the Fe(II)-2-oxoglutarate complex).

LEGENDS TO FIGURES.

Figure 1: the biosynthetic pathway to the penicillins and cephalosporins.

Figure 2 is a view of the active site of DAOCS showing 2-oxoglutarate binding to the iron and proposed penicillin N binding. Interactions with the side chains of certain amino acid residues are indicated by arrows.

Structure A is a three-dimensional structure of DAOCS.

Structure B is a high resolution crystal structure for prokaryotic DAOCS from *S. clavuligerus* as a complex with Fe(II) and 2-oxoglutarate.

The peptide sequence of DAOCS (with the numbering used herein) is set out below:

	Met	Asp	Thr	Thr	Val	Pro	Thr	Phe	Ser	T.e.n	10
									Gln		20
									Lys	_	30
								_	Leu	-	40
5									Asp		50
									Ser		60
									Pro		70
									Gly		80
	Glu	Ser	Glu	Ser	Thr	Ala	Gln	Ile	Thr	Asn	90
10	Thr	Gly	Ser	Tyr	Ser	Asp	Tyr	Ser	Met	Cys	100
	Tyr	Ser	Met	Gly	Thr	Ala	Asp	Asn	Leu	Phe	110
	Pro	Ser	Gly	Asp	Phe	Gly	Arg	Ile	Trp	Thr	120
	Gln	Tyr	Phe	Asp	Arg	Gln	Tyr	Thr	Ala	Ser	130
	Arg	Ala	Val	Ala	Arg	Glu	Val	Leu	Arg	Ala	140
15	Thr	Gly	Thr	Glu	Pro	Asp	Gly	Gly	Val	Glu	150
	Ala	Phe	Leu	Asp	Cys	Glu	Pro	Leu	Leu	Arg	160
	Phe	Arg	Tyr	Phe	Pro	Gln	Val	Pro	Glu	His	170
	Arg	Ser	Ala	Glu	Glu	Gln	Pro	Leu	Arg	Met	180
	Ala	Pro	His	Tyr	Asp	Leu	Ser	Met	Val	Thr	190
20	Leu	Ile	Gln	Gln	Thr	Pro	Cys	Ala	Asn	Gly	200
	Phe	Val	Ser	Leu	Gln	Ala	Glu	Val	Gly	Gly	210
	Ala	Phe	Thr	qzA	Leu	Pro	Tyr	Arg	Pro	Asp	220
	Ala	Val	Leu	Val	Phe	Cys	Gly	Ala	Ile	Ala	230
	Thr	Leu	Val	Thr	Gly	Gly	Gln	Val	Lys	Ala	240
25	Pro	Arg	His	His	Val	Ala	Ala	Pro	Arg	Arg	250
	Asp	Gln	Ile	Ala	Gly	Ser	Ser	Arg	Thr	Ser	260
	Ser	Val	Phe	Phe	Leu	Arg	Pro	Asn	Ala	Asp	270
	Phe	Thr	Phe	Ser	Val	Pro	Leu	Ala	Arg	Glu	280
	Cys	Gly	Phe	Asp	Val	Ser	Leu	Asp	Gly	Glu	290
30	Thr	Ala	Thr	Phe	Gln	Asp	Trp	Ile	Gly	Gly	300
	Asn	Tyr	Val	Asn	Ile	Arg	Arg	Thr	Ser	Lys	310
	Ala										311

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STRUCTURE A

CRYST1	106.400	106.40	0	71.100		90.00	90.00	120.00
SCALE1	0.009	9398	0.00542	6	0.0000	00	0.0000	00
SCALE2	0.000	0000	0.01085	2	0.0000	00	0.0000	00
SCALE3	0.000	0000	0.00000	0	0.0140	35	0.0000	00

- 13 -

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ATOM
        1
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                           31.434
                                    10.641
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ANISOU 1
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ATOM
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             C.A.
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                                    11.769
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ANISOU
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                       1
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                                                    -786
                                                          -1026 - 296
ATOM
        3
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                           30.472
                                    12.900
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ANISOU 3
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ATOM
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ANISOU 4
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                       1
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                                            4377
                                                    -402
                                                          -1097
ATOM
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                 AMET
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                                    11.328
                                            58.023 0.542 34.85
ANISOU 5
             CB
                 AMET
                           7877
                       1
                                    3692
                                            1672
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MOTA
        6
             CG
                 AMET
                       1
                           28.626
                                            57.903 0.542 38.19
                                    12.015
ANISOU
        6
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                       1
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MOTA
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ATOM
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ATOM
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- 14 -ANISOU 31 OD1 BASP 2 6276 4203 8095 -1203 3147 -1901 ATOM 32 OD2 BASP 2 29.760 18.945 59.875 0.732 34.85 ANISOU 32 OD2 BASP 2 2852 3708 6680 -491 444 -1450 ATOM 33 N THR 3 27.717 14.789 60.606 1.000 35.58 ANISOU 33 Ν THR 3 4586 4123 4811 601 -1628 1516 ATOM 34 CATHR 3 26.303 14.433 60.495 1.000 40.48 ANISOU 34 CA THR 3 4650 4555 6175 371 -911 - 385 MOTA 35 С THR 3 25.382 15.647 60.611 1.000 39.82 ANISOU 35 С THR 3 4376 4155 6598 320 -3864 -586 MOTA 36 0 THR 3 24.150 15.556 60.751 1.000 33.55 ANISOU 36 0 THR 3 4668 3107 4972 357 -2748 -588 MOTA 37 CB THR 25.905 13.450 61.613 1.000 39.95 3 ANISOU 37 CB THR 3 3787 4004 7387 160 -1209 6 2 OG1 THR ATOM 38 3 13.851 62.817 1.000 61.83 26.591 ANISOU 38 OG1 THR 3 10134 5882 7476 -4164 -3020 2051 ATOM 39 CG2 THR 3 26.399 12.052 61.278 1.000 59.32 ANISOU 3) CG2 THR 3 4613 3971 13955 1114 -3135 -198 ATOM 40 N THR 4 26.036 16.780 60.456 1.000 32.55 ANISOU 40 N THR 4 4306 4611 3450 377 -2166 -217 ATOM 41 CA THR 25.439 4 18.092 60.393 1.000 31.22 ANISOU 41 CA THR 4 4275 4229 3358 -81 -1179 9 5 ATOM 42 С THR 4 24.672 18.272 59.090 1.000 30.06 ANISOU 42 C THR 4 4876 3341 3207 773 -1156 -204 ATOM 43 0 THR 4 25.195 17.935 58.017 1.000 31.64 ANISOU 43 0 THR 4 4877 3780 1935 3363 -1255 - 52 ATOM 44CB THR 4 19.208 60.407 1.000 32.31 26.510 ANISOU 44 CB THR 4 2320 4762 5194 475 -547 5 9 3 ATOM 45 OG1 THR 227.324 4 19.091 61.578 1.000 32.36 ANISOU 45 OG1 THR 4 3705 3955 4635 -79 -797 - 389 ATOM 46 CG2 THR 4 25.852 60.458 1.000 27.22 20.582 ANISOU 46 CG2 THR 4 3728 4174 2443 71 304 - 151 MOTA 47 N VAL 5 23.464 18.796 59.211 1.000 21.69 ANISOU 47 N VAL 5 4041 1985 2215 -543 -657 1 5 8 ATOM CA VAL 48 5 22.690 19.140 58.024 1.000 20.42 ANISOU 48 CA VAL 5 3675 1964 2120 -622 -517 1 0 3 ATOM 49 С VAL 5 23.199 20.489 57.499 1.000 17.01 ANISOU 49 C VAL 5 2263 1803 2396 -279 -622 8 9 ATOM 50 0 VAL 5 23.156 21.449 58.252 1.000 21.10 ANISOU 50 0 VAL 5 3662 1885 2472 -389 -656 1 6 ATOM CB VAL 51 5 21.204 19.216 58.402 1.000 24.22 ANISOU 51 CB VAL 5 3551 2155 3495 -1045 -396 783 ATOM 52 CG1 VAL 5 20.434 19.700 57.166 1.000 20.14 ANISOU 52 CG1 VAL 5 3202 1779 2672 -453 10 -226 ATOM 53 CG2 VAL 5 20.701 17.867 58.860 1.000 28.58 ANISOU 53 CG2 VAL 5 5258 2086 3516 -1226 431 510 ATOM 54 N PRO 6 23.750 20.542 56.300 1.000 16.95 ANISOU 54 N PRO 6 2378 1629 29 -594 301 2434 CA PRO ATOM 55 6 24.354 21.793 55.857 1.000 16.90 ANISOU 55 6 1645 1775 3000 6 -445 303 56 ATOM C PRO 6 23.298 22.800 55.383 1.000 15.61 ANISOU 56 С PRO 6 1477 1766 2687 -192 -437 5 4 5 ATOM 57 0 PRO 6 22.133 22.432 55.201 1.000 15.75 ANISOU 57 0 PRO 6 1578 1761 2647 -260 -579 5 5 ATOM 58 СВ PRO 6 25.216 21.375 54.682 1.000 19.85 ANISOU 58 CB PRO 6 2320 1752 3468 50 70 1 8 2 ATOM 59 CGPRO 6 24.632 20.095 54.187 1.000 24.76 ANISOU 59 CG PRO 6 3550 2953 2904 -1186 300 - 286 ATOM 60 CD PRO 6 23.926 19.428 55.357 1.000 17.91 ANISOU 60 CD PRO б 1960 1962 2882 -168 -138 - 44 MOTA 61 N THR 7 23.723 55.156 1.000 14.38 24.031 ANISOU 61 THR 7 1518 1567 2378 -158 -616 1 0 0

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- 17 -ATOM 123 NE2 GLN 14 18.398 30.513 41.349 1.000 23.60 ANISOU 123 NE2 GLN 14 3058 2969 2941 -383 54 2 4 5 ATOM 124 GLN 15 M 25.309 31.243 41.395 1.000 25.00 ANISOU 124 GLN 15 M 3078 3281 3140 -1159 -394 5 7 5 MOTA 125 CAGLN 15 26.530 31.936 40.945 1.000 24.05 ANISOU 125 CAGLN 15 2947 3560 2631 -866 -98 655 ATOM 126 C 15 27.650 GLN 30.920 40.707 1.000 26.06 ANISOU 126 15 GLN 3810 2139 3951 -345 406 668 ATOM 127 0 GLN 15 28.756 31.284 40.302 1.000 35.85 ANISOU 127 0 GLN 15 4294 4851 4476 102 1871 1192 128 MOTA СВ GLN 15 27.018 32.918 42.009 1.000 25.90 ANISOU 128 СВ GLN 15 3055 3037 3748 -1092 -109 3 6 4 MOTA 129 CG GLN15 26.103 34.092 42.219 1.000 31.24 ANISOU 129 CG GLN 15 4562 2577 4731 -806 962 1054 ATOM 130 CDGLN 1.5 26.503 35.022 43.348 1.000 59.75 ANISOU 130 CD GLN 2475 15 9927 10301 -1855 -14 -1904 MOTA 131 OE1 GLN 15 35.031 43.840 1.000 81.81 27.634 ANISOU 131 OE1 GLN 15 3931 15059 12094 -944 -6272 -1803 ATOM 132 NE2 GLN 15 25.539 35.841 43.767 1.000 91.46 ANISOU 132 NE2 GLN 15 14070 4846 15833 -923 3672 -4850 ATOM 133 Ν GLY 16 27.379 29.643 40.969 1.000 29.90 ANISOU 133 Ν GLY 16 4634 3820 2907 -239 22 7 8 7 ATOM 134 CAGLY16 28.410 23.649 40.699 1.000 28.76 ANISOU 134 CAGLY 16 4466 3629 2833 -709 461 250 ATOM 135 C GLY 16 29.339 28.473 41.878 1.000 27.60 ANISOU 135 C GLY 16 3816 3779 2891 -616 914 1485 ATOM 136 0 GLY 16 30.398 27.867 41.725 1.000 31.47 ANISOU 136 0 GLY 16 3386 4758 3814 -899 1243 1023 ATOM 137 LEU Ν 17 28.960 28.898 43.083 1.000 26.01 ANISOU 137 Ν LEU 17 3295 2950 3636 -721 162 743 ATOM 138 CALEU 17 29.776 28.666 44.257 1.000 23.96 ANISOU 138 CALEU 17 2700 3032 3372 -601 100 673 ATOM 139 С LEU 17 29.462 27.338 44.932 1.000 20.31 ANISOU 139 C LEU 17 2222 2763 2733 -252 611 261 ATOM 140 0 LEU 17 28.389 26.780 44.789 1.000 23.13 ANISOU 140 0 LEU 17 2347 3134 3308 -443 263 859 ATOM 141 СB LEU 17 29.645 45.286 1.000 25.94 29.806 ANISOU 141 CB LEU 17 2886 2933 4035 -1318 -405 2 5 4 ATOM 142 CG LEU 44.716 1.000 31.57 17 29.962 31.209 ANISOU 142 CG LEU 17 3741 2948 5308 -523 1150 7 2 2 ATOM 143 CD1 LEU 17 29.550 32.358 45.615 1.000 32.04 ANISOU 143 CD1 LEU 17 5221 2887 4066 -1269 278 508 ATOM 144 CD2 LEU 17 31.458 31.278 44.416 1.000 38.11 ANISOU 144 CD2 LEU 17 3828 5491 5160 -2315 954 ATOM 145 N HIS 18 30.441 26.822 45.681 1.000 22.49 ANISOU 145 N HIS 18 2600 3067 2877 -662 42 4 4 9 ATOM 146 CAHIS 18 30.289 46.537 1.000 21.54 25.644 ANISOU 146 CAHIS 18 2378 2809 2996 -432 201 ATOM 147 С HIS 18 29.908 24.376 45.790 1.000 22.76 ANISOU 147 C HIS 18 2256 3245 3148 -1009 282 ATOM 148 0 HIS 18 29.147 23.565 46.331 1.000 22.60 ANISOU 148 0 HIS 18 2008 3064 3516 -629 -166 8 8 4 ATOM 149 СВ HIS 18 25.872 47.618 1.000 22.81 29.224 ANISOU 149 СЗ HIS 18 2514 2879 3272 -526 450 421 ATOM 150 CG HIS 18 29.320 27.248 48.217 1.000 21.70 ANISOU 150 CG HIS 18 2797 3038 39 5 0 3 2411 -149 ATOM 151 ND1 HIS 18 30.438 27.773 48.807 1.000 25.01 ANISOU 151 ND1 HIS 18 3714 3505 2284 -207 -629 1 4 9 ATOM 152 CD2 HIS 18 28.370 28.216 48.269 1.000 24.95 ANISOU 152 CD2 HIS 18 3244 3278 2957 87 544 2 7 5 ATOM 153 CE1 HIS 18 30.197 28.982 49.223 1.000 29.26

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- 18 -
  ANISOU 153
               CE1 HIS
                       18 4603
                                    3396
                                            3118
                                                  -388 -335 2 7
          154
                       18 28.937 29.271 48.919 1.000 27.24
               NE2 HIS
  ANISOU 154
               NE2 HIS
                       18
19
                           4582
                                    3137
                                            2632
  ATOM
                            30.269 24.270 44.521 1.000 22.74
                                                    2 224 3 6 5
          155
               N
                   GLN
  ANISOU 155
                       19
               N
                   GLN
                            2724
                                    3094
                                            2822
  ATOM
                                                   -511 -123 4 2 3
          156
               CA GLN
                            29.806 23.113 43.730 1.000 23.85
                        19
  ANISOU 156
              CA GLN
                        19
                            3129
                                    2668
                                            3263
  ATOM
         157
                                                    148 63 8 9
                            30.271 21.760 44.221 1.000 22.77
                   GLN
                        19
  ANISOU 157
               С
                  GLN
                       19
                            2532
                                    3026
                            29.480 20.801 44.259 1.000 21.99
1869 2911 3574 -187 0 558
                                            3095
                                                   -502 -574 778
  ATOM
         158
              0
                  GLN
                       19
  ANISOU 158
              0
                  GLN
                       19
  ATOM
         159
              СВ
                            30.227 23.322 42.276 1.000 27.66
                 GLN
                       19
  ANISOU 159
              CВ
                  GLN
                       19
                            5043
                                    2519
                                            2947
  ATOM
                                                   29 -339 458
                           29.397 24.333 41.523 1.000 26.21
         160
              CG
                  GLN
                       19
 ANISOU 160
              CG
                  GLN
                       19
                            3289
                                    3163
                                           3508
  ATOM
                                                   299
         161
              CD
                                                         171 437
                  GLN
                       19
                           27.917
                                   24.368 41.862 1.000 32.47
 ANISOU 161
              CD
                  GLN
                       19
                           3403
                                    4411
                                           4521
 ATOM
                                                   -986 535 654
         162
              OE1 GLN
                       19
                           27.154
                                   23.604 41.277 1.000 39.69
 ANISOU 162
              OE1 GLN
                       19
                           ATOM
                                                   -262 -2770 1829
         163
             NE2 GLN
                       19
 ANISOU 163
             NE2 GLN
                       19
                           3803
                                   6153
 ATOM
                                           6212
                                                   81 1944 1 1
         164 N
                  ASP
                       20
                                   21.572 44.631 1.000 22.63
                           31.526
 ANISOU 164 N
                  ASP
                       20
                           2073
                                   3400
                                           3123
 ATOM
         165 CA ASP
                                                   -414 95 708
                       20
                           31.926
ANISOU 165 CA
ATOM 166 C ASP
ANISOU 166 C ASP
ATOM 167 O ASP
ANISOU 167 O ASP
ATOM 168 CB ASP
CP ASP
 ANISOU 165 CA ASP
                                          45.225 1.000 23.10
                                   20.292
                       20
                           1869
                                   3674
                                           3235
                                                   83 236 7 0 4
                       20
                           31.190 20.042
                                          46.546 1.000 20.03
                 ASP
                       20
                           1775
                                   2963
                                           2873
                                                   -280 -143 4 9 3
                       20 30.772 18.899 46.768 1.000 21.48
20 1429 2884 3848 -311 225 2
                                                         225 224
                          33.414 20.268 45.521 1.000 27.66
                       20
 ANISOU 168
             CB ASP
                       20 1835
                                   4546
                                           4130
 ATOM
                                                  -16
        169
             CG
                       20 34.298 20.206 44.291 1.000 39.35
                                                         207 881
                 ASP
 ANISOU 169
                 ASP
             CG
                       20 2355
                                   6893
 ATOM
                                           5705
                                                  -654 1323 -1915
        170
                       20 33.870 19.914 43.153 1.000 35.78
             OD1 ASP
 ANISOU 170
             OD1 ASP
                       20 3152.
                                  5452
                                           4992
 MOTA
                                                  -741 1508 - 797
        171
             OD2 ASP
                       20 35.508 20.433
20 2201 8705
                                          44.467 1.000 45.22
 ANISOU 171
             OD2 ASP
MOTA
                                           6277
                                                  -589
        172
                                                        1088 - 87
             N
                 GLU
                       21 31.046 21.053
ANISOU 172
                                           47.404 1.000 20.01
             Ν
                      21 1574
                 GLU
                                  2935
                      21 30.323 20.811 48.665 1.000 18.97
21 1412 2956 2838 -481 -464 1
21 28.858 20.448 48.402 1.000 17.84
21 1386 2342 3050 -307 -395 2
21 28.290 19.602 49.054 1.000 18.46
                                           3093
                                                  -412 -241 3 6 7
ATOM
        173
             CA GLU
ANISOU 173
             CA GLU
                                           2838 -481 -464 1 1 8
ATOM
        174
                 GLU
ANISOU 174
             С
                 GLU
ATOM
                                                  -307 -395 2 3 4
        175
             0
                 GLU
ANISOU 175
             0
                 GLU
                         1671
                                  2286
                                          3057
                                                  -419 -351 1 1 6
ATOM
        176
             CB
                         30.415 22.058 49.563 1.000 20.10
                 GLU
                      21
ANISOU 176
             CВ
                 GLU
                         1646
                      21
                                  2821
                                          3170
ATOM
                                                  -514 -499 1 2 7
        177
             CG
                 GLU
                         31.893 22.322
                      21
                                          49.918 1.000 24.11
ANISOU 177
             CG
                 GLU
                      21
                         1682
                                  3568
ATOM
                                          3912
                                                  -766 -326 -711
        178
             CD
                 GLU
                      21
                         32.574
                                  23.380
ANISOU 178
                                          49.081 1.000 29.70
             CD
                 GLU
                      21
                         1330
                                  4241
                                          5713
ATOM
                                                  -752 -666 5 2 1
       179
             OE1 GLU
                      21
                         32.249 23.594
                                          47.887 1.000 35.14
ANISOU 179
             OE1 GLU
                      21
                          2623
                                  4054
                                          6677
                                                  -1336 -1741 1977
ATOM
       180
            OE2 GLU
                      21
                          33.483 24.007
                                         49.678 1.000 39.39
ANISOU 180
            OE2 GLU
                      21.3681
                                  4425
                                          6860
ATOM
                                                  -2089 -1618 647
       181
            N
                 PHE
                      22
                          28.231 21.048
ANISOU 181
                                          47.395 1.000 17.30
            M
                 PHE
                      22
                          1540
                                  2352
MOTA
                                          2680
                                                 -243 -446 - 79
       182
            CA
                PHE
                      22
                          26.851 20.761
ANISOU 182
                                          47.071 1.000 17.13
            CA
                PHE
                      22
                          1534
                                  2166
ATOM
                                          2807
       183
            С
                                                 -235 -396 3 7 4
                          26.733 19.329 46.552 1.000 17.41
                PHE
                      22
ANISOU 183
            C
                PHE
                      22
                         1688
                                  2500
                                          2427
                                                 -502 -334 1 0 4
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O PHE 22 25.867 18.574 46.995 1.000 15.87 O PHE 22 1570 2118 2343 -249 ATOM 184 0 ANISOU 184 0 2343 -249 -361 1 3 1 ATOM 185 26.305 21.840 46.149 1.000 18.00 ANISOU 185 CB PHE 22 1747 2754 2337 70 -178 445 24.802 21.729 45.930 1.000 16.38 1747 MOTA 186 CG PHE 22 ANISOU 186 CG PHE 22 1763 2714 -90 1748 -326 2 2 3 CD1 PHE MOTA 187 22 23.934 21.723 47.003 1.000 18.29 ANISOU 187 CD1 PHE 22 1812 2091 3045 -197 -88 576 ATOM CD2 PHE 188 22 24.290 21.720 44.641 1.000 18.62 ANISOU 188 CD2 PHE 22 2106 2079 2890 -143 -623 3 9 4 ATOM 189 CE1 PHE 22 22.569 21.727 46.771 1.000 18.90 ANISOU 189 CE1 PHE 22 1826 2086 3271 -198 -133 3 0 2 ATOM 190 CE2 PHE 22 22.911 21.660 44.379 1.000 19.28 ANISOU 190 CE2 PHE 22 2189 2023 3114 -242 -754 - 144 191 CZPHE 22 22.059 21.645 45.473 1.000 19.42 ANISOU 191 CZPHE 22 2048 1723 3607 90 -483 -376 192 N ARG 23 27.580 18.971 45.583 1.000 17.88 ANISOU 192 Ν ARG 23 1647 2437 2709 -168 -218 3 1 7 MOTA 193 CA ARG 23 27.520 17.594 45.079 1.000 19.18 ANISOU 193 CA ARG 23 1724 2539 3022 -166 36 1 5 8 ATOM 194 ARG 23 27.767 16.595 46.211 1.000 19.11 ANISOU 194 C ARG 23 1279 2461 3518 -173 -113 4 5 5 ATOM 195 0 ARG 23 27.107 15.547 46.229 1.000 18.82 ANISOU 195 0 ARG 23 1614 2156 3381 -33 181 - 128 ATOM 196 CB ARG 23 28.605 17.351 44.030 1.000 22.81 ANISOU 196 CB ARG 23 1934 4099 2633 -34 -105 - 354ATOM 197 CG ARG 23 28.248 17.790 42.617 1.000 24.82 ANISOU 197 CG ARG 23 2601 4078 2752 191 -122 - 204 ATOM 198 CD ARG 23 ²29.376 17.272 41.685 1.000 29.71 ANISOU 198 CDARG 23 2503 5619 3168 -285 908 704 MOTA 199 NE ARG 30.479 18.206 23 41.800 1.000 30.96 ANISOU 199 ΝE ARG 23 2877 5034 3851 -43 286 ATOM 200 CZARG 23 30.549 19.360 41.148 1.000 ?9.49 ANISOU 200 CZ ARG NH1 ARG 23 2612 5063 3529 -225 606 ATOM 201 23 29.536 19.665 40.328 1.000 29.26 ANISOU 201 NH1 ARG 23 3242 4951 2923 -960 331 525 ATOM 202 NH2 ARG 31.629 20.092 41.345 1.000 32.61 23 ANISOU 202 NH2 ARG 23 2320 5347 4722 -134 519 179 ATOM 203 28.708 16.851 47.125 1.000 17.80 N ARG 24 ANISOU 203 N 1262 2168 3332 183 38 9 8 28.930 15.899 48.222 1.000 18.85 ARG 24 ATOM 204 CA ARG 24 1368 2509 3287 69 -162 1 0 1 27.701 15.811 49.114 1.000 17.51 ANISOU 204 CA ARG 24 3287 69 -162 105 ATOM 205 С ARG 24 ANISOU 205 C ARG 24 -177243ATOM 206 O ARG 24 ANISOU 206 0 ARG 1851 1965 2997 -16 -402 2 30.203 16.321 48.991 1.000 19.88 24 -402 2 5 3 ATOM CB ARG 207 24 ANISOU 207 CB ARG 1685 2700 3169 -398 -218 4 31.459 16.053 48.135 1.000 29.07 24 3169 -398 -218 4 ATOM 208 CG ARG 24 ANISOU 208 CG ARG 24 1467 4625 4954 269 203 709 ATOM 209 CD ARG 32.700 16.206 24 49.016 1.000 41.84 ANISOU 209 CD ARG 24 1745 7021 7130 -451 -494 -922 ATOM 210 NE ARG 33.690 17.103 24 48.464 1.000 57.06 ANISOU 210 NE ARG 24 4362 8003 -3326 -669 -1141 9316 ATOM 211 34.032 18.327 CZARG 24 48.810 1.000 60.67 ANISOU 211 CZ ARG 5961 24 10369 6723 -4627 -1324 -1586 ATOM 212 NH1 ARG 33.430 18.980 24 49.799 1.000 49.70 ANISOU 212 NH1 ARG 24 7748 6565 4569 -951 -2185 2226 ATOM 213 NH2 ARG 24 34.997 18.971 48.159 1.000 54.12 ANISOU 213 NH2 ARG 8696 8490 3378 -3780 -2352 1607 27.092 16.963 49.370 1.000 15.74 24 ATOM 214 Ν CYS 25

								PC 1/GB98/03860
	SOU 2		ı CY	S 25	1435	- 20 -		
ATOM		15 (CA CY			1969	2574	-16 -393 - 33
	SOU 2:		A CY			34 16.92 1954		3 1.000 16.39
ATOM	1 2. 500 2:	16 (24.82	6 16.06	2756	-95 -317 - 300
ATOM	1 21	_			1629	1699	2648	7 1.000 15.73
	OU 21	l7 c l7 c				4 15.26	2 50.155	-114 -432 6 6 5 1.000 15.89
ATOM		_	B CY			1801	2783	-88 -469 2 5 2
ANIS	OU 21	.8 <u> </u>	B CY		25.36 1644		2 50.424	1.000 15.93
ATOM			G CY		23.70	1779	2029	-49 -261 20
ANIS ATOM		_		S 25	1742	0 18.41 1825		1.000 17.82
	22 0U 22	_			24.62	3 16.30	3202 8 48.250	-122 -33 -55
ATOM					1449	1843	2504	
ANIS	วช 22				23.56		47.534	$ \begin{array}{rrr} -54 & -263 - 142 \\ 1.000 & 15.62 \end{array} $
ATOM	22	2 C	LEU		1616 23:763	1739	258U	-86 -453 4 0
ANISO ATOM	OU 22	_	LFU		1697	3 14.085 1764		1.000 15.18
ANISC	22.		LEU		22.819	13.345	2306	-113 -479 6
ATOM	22		LEU		1797	1725	2920	1.000 16.96
ANISC	U 224	1 CF			23.526		46.066	-234 -664 -300 1.000 16.02
ATOM	225	c c	-~0		1811 23.057	1645	4633	-191 - 483122
ANISO ATOM			LEU	26	1762	17.510 1716		1.000 15 60
ANISO	226 U 226		1 LEU		23.252	17.880	4485	-6 -15 7 9
ATOM	227		1 LEU 2 LEU	_	1750	2360	2532	1.000 17.48 -17 -130 465
ANISO	U 227	CD	2 LEU	26 26	21.584 1655		46.290	1.000 17.11
ATOM	228	N	ARG		25.027	2188 13.648	205U	-29 <u>-</u> 75 1 c o
ANISO: ATOM	0 228 229		ARG	21	1870	1818	47.494 2871	1.000 17.26 155 -326 1 4 0
ANISO	J 229	CA CA	ARG ARG	27	25.295	12.205	47.372	155 -326 1 4 0 1.000 18.75
\mathtt{ATOM}	230	C	ARG	27 27	2108 25.240	1845	31/U	270 - 955 102
ANISOU ATOM	J 230	C	ARG	27	1667	11.599 1801	48.744	1.000 17.95
ANISOL	231	0	ARG	27	24.777	10.454		159 -897 2 1 9
ATOM	232	O CB	ARG ARG		2158	1793		1.000 20.99 -43 -360 1 6 8
ANISOU	7 232	CB	ARG	27 27	26.641 2815	12.008	46.670	1.000 21.35
ATOM	233	N	ASP		25.827	2034 12.293	3264 + 6	522 -377 - 129
ANISOU ATOM	233	N	ASP	28	1487	2004	49.723 1 2856 1	1.000 16.71
ANISOU	234	CA CA	ASP ASP	28	26.034	11.672	51.026 1	178 -328 6 7 1.000 17.47
ATOM	235	C	ASP	28 28	1613	2095	2931 1	.07 -301 1 2 2
ANISOU	235	С	ASP		24.872 1414	11.866 2264	51.990 1	000 17.22
ATOM ANISOU	236	0	ASP	28	24.816	11.081	2803 2	23 -447 4 7 1
ATOM	237	O CB	ASP ASP	28	1932	2139		.000 17.62 50 -565 3 2 7
ANISOU	237	CB	ASP	28 ;	27.306	12.237	51.657 1	50 -565 3 2 7 .000 22.17
ATOM	238	CG	ASP		1581 28.590	3894	2948 -	272 -467 5 5 a
ANISOU ATOM	238 239	CG	ASP	28	1596	11.906 3323	50.941 1 4472 2	.000 24.72
ANISOU	239	OD1	ASP ASP	28 2	28.572	10.905	50 199 1	36 -288 6 4 8 .000 27.56
\mathtt{ATOM}	240	OD2	ASP		2317	3071	5084 8	08 -284 5 7 2
ANISOU	240	OD2	ASP	_	29.573 1584	12.617	51.251 1	.000 32.08
ATOM ANISOU	241	N	LYS		24.098	4343 12.942	6261 -	144 -470 4 1 6
ATOM	241 242	И СА	LYS	29 1	.475	1814	51.821 1 2627 5	.000 15.57
ANISOU	242	CA	LYS LYS	29 2 29 1	3.048	13.305	52.778 1	-303 178 .000 15.13
ATOM	243	С	LYS		.584 1.686	1999	2165 -	68 -500 - 96
ANISOU ATOM	243	C	LYS	_	496	13.500 1352	52.118 1	.000 14.56
ANISOU	244		LYS	29 2	0.688		2686 7	7 -452 106
=	~ 4 4	0	LYS	29 1				.000 16.21 177 -315 - 5
							•	

- 21 -MOTA 245 CВ LYS 23.431 29 14.563 53.574 1.000 16.09 ANISOU 245 СВ LYS 29 1666 1672 2777 3 -642 - 25 MOTA 246 CG LYS 29 24.776 14.421 54.292 1.000 17.68 ANISOU 246 CG LYS 29 1918 2192 7 -1144 141 2606 ATOM 247 CDLYS 29 25.161 15.647 55.096 1.000 20.71 ANISOU 247 CD LYS 29 2675 2044 3151 -35 -1518 4 1 ATOM CE 248 LYS 29 26.498 15.331 55.844 1.000 22.24 ANISOU 248 CE LYS 29 2203 2714 3535 142 ~1369 - 685 ATOM 249 NZLYS 29 26.955 16.594 56.492 1.000 32.67 ANISOU 249 NZLYS 29 5831 3199 3381 -502 -2085 -1260 ATOM 250 Ν GLY 14.198 50.993 1.000 14.09 3 0 21.604 GLY ANISOU 250 M 30 1552 2340 1461 135 -455 - 100 251 CAGLY 3 0 20.358 14.373 50.250 1.000 14.09 ANISOU 251 CAGLY30 1428 1561 2365 92 - 342 - 97 ATOM 252 С GLY 30 19.372 15.284 50.955 1.000 12.30 ANISOU 252 С GLY 30 1423 1192 2059 -95 -275 9 4 ATOM 253 GLY 30 18.168 15.223 50.696 1.000 14.58 ANISCU 253 0 GLY 30 1435 1689 2415 52 -476 -121 ATOM 254 31 N LEU 19.884 16.146 51.823 1.000 13.93 ANISOU 254 N LEU 31 1472 1479 2343 -182 -248 -181 ATOM 255 CA LEU 31 19.012 17.114 52.511 1.000 14.44 ANISOU 255 CALEU 31 1534 1457 -235 -55 -246 2495 ATOM 256 С LEU 31 19.894 18.286 52.942 1.000 15.08 ANISOU 256 C LEU 31 1411 1535 2784 -177 -326 - 314ATOM 257 0 LEU 31 21.113 18.136 53.140 1.000 15.64 ANISOU 257 0 LEU 31 1468 1664 2812 -328 - 67-169 MOTA 258 CB LEU 31 18.222 16.560 53.694 1.000 16.76 ANISOU 258 СB LEU .2192 31 1664 2511 -367 128 - 213 ATOM 259 CG LEU 18.883 16.517 31 55.039 1.000 20.16 ANISOU 259 LEU CG • 31 2435 2485 2739 -289 -141 4 4 5 ATOM 260 CD1 LEU 31 17.977 16.145 56.202 1.000 26.49 ANISOU 260 CD1 LEU 31 2253 5076 2738 -508 -341 9 6 9 ATOM 261 CD2 LEU 31 20.052 55.032 1.000 24.73 15.526 ANISOU 261 CD2 LEU 31 4192 2967 2237 1001 153 610 ATOM 262 Ν PHE 32 19.289 19.462 53.052 1.000 14.11 ANISOU 262 И PHE 32 1569 1457. 2335 -231 -179 - 207ATOM 263 CA PHE 20.020 20.697 32 53.417 1.000 13.56 ANISOU 263 CA PHE 32 1447 1389 2317 -225 ATOM 264 С PHE 32 18.976 21.777 53.687 1.000 13.72 ANISOU 264 С PHE 32 1411 1439 2365 -218 -421 -142 ATOM 265 0 PHE 32 17.889 21.711 53.118 1.000 15.50 ANISOU 265 0 PHE 32 1392 1862 2634 -175 -436 - 389 ATOM 266 CB PHE 32 20.958 21.157 52.308 1.000 15.01 ANISOU 266 CB PHE 32 1379 2201 2125 -305 -342231MOTA 267 CG PHE 32 20.381 21.156 50.920 1.000 14.60 ANISOU 267 CG PHE 32 1649 1662 2237 -193 -429 1 1 8 ATOM CD1 PHE 268 32 50.148 1.000 14.53 20.326 19.986 ANISOU 268 CD1 PHE 32 1328 1688 2504 -156 -507 1 5 ATOM 269 CD2 PHE 19.831 32 22.345 50.396 1.000 13.66 ANISOU 269 CD2 PHE 32 1320 1678 2191 -179 -309 1 6 6 ATOM 270 CE1 PHE 32 19.742 20.033 48.892 1.000 14.26 ANISOU 270 CE1 PHE 32 1507 1655 2256 -346 -271 1 9 9 MOTA 271 CE2 PHE 32 19.267 22.348 49.138 1.000 15.49 ANISOU 271 CE2 PHE 32 1681 1932 2272 72 -504 -126 MOTA 272 CZ PHE 32 19.177 21.184 48.385 1.000 15.25 ANISOU 272 CZPHE 32 1979 1700 2117 -185 -295 1 6 8 ATOM 273 N TYR 33 19.376 22.785 54.442 1.000 14.44 ANISOU 273 N TYR 33 1813 1302 2372 -237 -496 - 50ATOM 274 CATYR 33 18.616 24.023 54.519 1.000 14.32 ANISOU 274 СA TYR 1764 33 1415 2261 -143 -295 - 111ATOM 275 С TYR 33 19.039 24.929 53.364 1.000 13.70

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- 22 -
 ANISOU 275
            С
                TYR 33
                         1479
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        276
            0
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                TYR
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 ANISOU 276
            0
                TYR
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 ATOM
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ATOM
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ATOM
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ANISOU 285 N
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ATOM
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MOTA
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ATOM
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ANISOU 294 CA THR
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                                1537
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                                              -206 -827 -196
ATOM
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               THR
                    3 5
                                31.127 51.010 1.000 17.04
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ANISOU 295 C
               THR
                    35
                        1895
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                                       2887
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       296 0
ATOM
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ANISOU 297
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ATOM
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ANISOU 298
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ATOM
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                                                  -1113 5 9
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ANISOU 300
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               ASP
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ANISOU 301
           CA ASP
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ATOM
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           C
               ASP
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ANISOU 302
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ATOM
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ATOM
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ANISOU 304
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                                2366
                                       3406
                                              -876 <del>-</del>755 8 0 7
ATOM
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               ASP
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ANISOU 305
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                        2537
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                                       4402
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- 23 -OD1 ASP 36 20.061 34.886 51.457 1.000 26.16 MOTA 306 ANISOU 306 OD1 ASP 3 6 2981 2100 4860 378 -777 - 381 307 OD2 ASP 36 21.824 33.982 50.528 1.000 24.87 ANISOU 307 OD2 ASP 36 1994 4924 -49 -950 -628 32.196 48.971 1.000 20.25 2532 ATOM 308 N CYS 3 7 16.282 ANISOU 308 3 7 1711 3849 118 -638 - 263 31.587 47.902 1.000 20.28 N CYS 2135 ATOM 309 CA CYS 37 15.463 ANISOU 309 CA CYS 37 2390 1478 3839 136 -799 - 138 14.078 32.183 47.818 1.000 19.90 ATOM 310 C CYS 37 ANISOU 310 C CYS 37 2374 1724 3463 214 -711 - 74 13.176 31.629 47.156 1.000 22.75 ATOM 311 O CYS 3 7 ANISOU 311 O CYS 37 ATOM 312 CB CYS 3 7 ANISOU 312 CB CYS 37 2739 1454 4247 194 -477 - 115 14.500 29.595 49.596 1.000 22.84 313 SG CYS ATOM 37 ANISOU 313 SG CYS ATOM 314 N GLY 37 2854 1884 3942 -203 -922 1 4 1 13.855 33.390 48.314 1.000 20.85 2854 1884 38 ANISOU 314 N GLY ATOM 315 CA GLY ANISOU 315 CA GLY ATOM 316 C GLY 38 2233 1874 4790 255 -292 1 6 5 38 11.534 33.619 49.217 1.000 23.29 ANISOU 316 C GLY 38 2577 2045 4228 113 -136 -601 38 10.400 34.091 49.129 1.000 25.58 ATOM 317 0 GLY ANISOU 317 0 ${ t GLY}$ 38 2529 3424 3765 214 -96 - 264 ATOM 39 11.894 32.836 50.237 1.000 24.55 39 2310 2980 4037 119 -46 -318 N LEU ANISOU 318 N LEU 4037 119 -46 -364 CA LEU 39 10.938 32.331 51.195 1.000 24.44 39 2637 2964 3684 -105 175 -39 11.107 32.885 52.593 1.000 35 41 ATOM 319 ANISOU 319 39 11.107 32.885 52.593 1.000 35.41 39 5341 4215 3898 700 757 3684 -105 175 -946 ATOM 320 C LEU ANISOU 320 C LEU 3898 -796 165 -1435 321 O LEU ATOM 39 11.784 32.313 53.441 1.000 43.41 ANISOU 321 O LEU 39 7338 4986 4171 -2639 - 1333 - 303322 CB LEU ATOM 39 10.850 30.810 51.206 1.000 26.48 ANISOU 322 CB LEU 39 4244 2940 2879 49 -70 - 261 CG LEU ATOM 323 39 10.404 30.097 49.921 1.000 30.21 ANISOU 323 CG LEU 39 4834 4195 2452. 258 -1618 -474 ATOM 324 CD1 LEU 39 28.595 49.972 1.000 24.78 10.683 ANISOU 324 CD1 LEU 39 3351 2597 3468 424 -707 - 30.407 49.640 1.000 27.50 424 -707 -118 ATOM 325 CD2 LEU 39 8.940 ANISOU 325 CD2 LEU 39 4828 2118 3503 860 -860 - 323 ATOM 326 N THR 40 10.365 33.957 52.882 1.000 45.58 ANISOU 326 N THR 40 7392 4849 -520 2852 -1993 5077 327 CA THR 40 10.610 34.661 54.136 1.000 32.50 ATOM ANISOU 327 CA THR 40 4224 3732 4393 999 961 - 558 ATOM 328 C THR 40 9.700 ANISOU 328 C THR 40 3175 34.177 55.248 1.000 29.68 4204 3898 -116 294 -1630 ATOM 329 O THR 33.556 55.031 1.000 39.75 40 8.653 ANISOU 329 O THR 40 3930 5847 5326 -1079 -301 -1653CB THR ATOM 330 40 10.641 36.183 53.997 1.000 56.31 ANISOU 330 40 10586 -1417 1006 - 992 3758 7052 ATOM 331 OG1 THR 40 11.545 36.606 52.946 1.000 68.39 ANISOU 331 OG1 THR 40 7379 3900 14707 -1978 3617 -246 ATOM CG2 THR 40 11.214 36.837 55.256 1.000 70.22 332 ANISOU 332 CG2 THR 40 8265 5228 13188 1389 -4422 -3241 ATOM 333 N ASP 41 10.191 34.302 56.486 1.000 33.20 N ASP 41 3580 CA ASP 41 9.329 CA ASP 41 2705 ANISOU 333 5223 3810 -203 307 -1779 ATOM 334 33.943 57.613 1.000 27.51 ANISOU 334 41 2705 3858 3891 91 -253 -1061 ATOM 335 С ASP 41 8.107 34.861 57.660 1.000 33.43 ANISOU 335 С ASP 41 3131 3064 6508 32 547 - 1307 ATOM 336 0 ASP 41 7.034 34.469 58.101 1.000 30.76

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- 24 -
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                         ASP 41 2690
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     ATOM 337 CB ASP 41 4853
ATOM 338 CG ASP 41 9.453
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9.453 33.351 60.039 1.000 33.37
                                                                   -1222 -698 -938
                              41 3324 5291 4065 -739 -501 -

41 9.152 32.164 59.780 1.000 34.95

41 9.395 33.904 61.161 1.000 86.76
                    CG ASP
     ATOM
              339
                    OD1 ASP
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    ANISOU 339
                    OD1 ASP
    ATOM
           340
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42 7.198 37.074 57.221 1.000 38.48
    ATOM 342
ANISOU 342
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                   CA THR
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    ATOM
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    ANISOU 343
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                        THR
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                        THR
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                  CB THR 42
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   ANISOU 345 CB THR 42 4526 3763 56.815 1.000 37.05
ATOM 346 OG1 THR 42 8.831 38.301 55.889 1.000 98.08
ATOM 347 CG2 THR 42 8.358 39.113 58.047 1.000 36.08
ATOM 348 N GIU 42 6097 3613 3997 886 -1119 2.69
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36.184 55.173 1.000 3 4.64
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GLU 43
GLU 43
GLU 43
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   ANISOU 348 N
                       GLU
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   ATOM
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  ANISOU 350
                 С
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           351 0
  ATOM
                      GLU
  ANISOU 351 O
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43 6.278 35.074 53.026 1.000 44.72
                      GLU
  ATOM
           352 CB GLU
  ANISOU 352 CB
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43 6.658 36.125 52.003 1.000 53.42
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  ATOM
          353
                CG
                      GLU
  ANISOU 353
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 ATOM 354
ANISOU 354
 ATOM
 ATOM 355
ANISOU 355
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 ATOM
 ANISOU 356
 ATOM
 ANISOU 357
 ATOM
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LEU 44 1930 4771 6333 -537 776 - 262

LEU 44 2046 5235 53.90 -840 705
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ANISOU 361
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ANISOU 362
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ATOM
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ANISOU 363
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ATOM
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33.712 57.694 1.000 41.91
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ATOM
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ANISOU 365 N
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                    LYS 45
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ANISOU 366 CA LYS
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- 25 -ATOM 367 LYS 45 1.981 34.582 58.278 1.000 33.58 ANISOU 367 C LYS 45 4535 3445 6681 -245 1221 - 2820 MOTA 368 0 LYS 45 0.984 34.238 58.902 1.000 39.93 ANISOU 368 0 LYS 4857 3594 6720 262 1634 - 2337 ATOM 369 CB LYS 4.038 35.400 59.447 1.000 50.20 ANISOU 369 СВ LYS 45 4944 5561 8569 1081 -447 -3980 MOTA 370 CG LYS 45 3.082 36.546 59.706 1.000 53.07 ANISOU 370 CG LYS 45 3548 6321 10296 1148 -2094 -4809 ATOM 371 CD LYS 45 3.714 37.922 59.622 1.000 58.29 ANISOU 371 CD LYS 45 4723 5694 11730 1422 -3745 -5024 ATOM 372 CE LYS 45 3.199 60.761 1.000 65.33 38.793 ANISOU 372 CE LYS 45 6294 6898 11629 -3430 -5603 1072 ATOM 373 NZLYS 45 1.713 38.779 60.852 1.000 73.75 ANISOU 373 ΝZ LYS 45 6392 9216 12412 -718 -1071 - 7436374 ATOM N SER 46 1.973 35.341 57.193 1.000 36.94 ANISOU 374 N 46 SER 4074 3478 6484 -956 1068 - 2939 375 MOTA CASER 46 0.743 35.856 56.607 1.000 37.61 ANISOU 375 CASER. 4 € 3983 6892 3417 -1335 988 -2335 ATOM 376 С SER 46 -0.137 34.702 56.137 1.000 34.45 ANISOU 376 С SER 46 3430 3057 -1104 1656 -2394 6602 377 ATOM 0 SER 46 -1.337 34.625 56.449 1.000 29.50 ANISOU 377 0 SER 46 3195 2789 5224 -587 1093 -1206 СВ 378 MOTA SER 46 1.160 36.726 55.419 1.000 40.36 ANISOU 378 СВ SER 46 4102 3809 7425 -2099 617 -1930 379 ATOM OG SER 46 0.018 37.017 54.630 1.000 43.38 ANISOU 379 0G SER 46 5005 8048 3431 -1261 53 -1863 ATOM 380 Ν ALA 47 0.493 33.808 55.361 1.000 29.82 ANISOU 380 N ALA 47 3246 2173 5910 -18 809 -1228 CA ALA ATOM 381 47 -0.208 32.623 54.879 1.000 25.84 ANISOU 381 CA ALA 47 3566 2106 4148 7 630 - 891 ATOM 382 С ALA 47 -0.722 31.792 56.058 1.000 25.02 ANISOU 382 С ALA 47 2591 2344 4572 481 280 - 280 ATOM 383 0 ALA 47 -1.838 56.063 1.000 23.19 31.381 ANISOU 383 0 ALA 47 2850 2366 3597 129 318 -1119 ATOM 384 CВ ALA47 53.912 1.000 26.76 0.615 31.791 ANISOU 384 СВ ALA 47 2892 2764 4511 270 351 -1134 ATOM 385 LYS N 48 0.132 31.529 57.041 1.000 24.64 ANISOU 385 Ν LYS 48 3107 2076 4178 130 -57 -1085 ATOM 386 CALYS 48 -0.186 30.712 58.202 1.000 25.83 ANISOU 386 CALYS 48 3545 2979 3291 -16 30 - 1416 ATOM 387 C LYS 48 -1.33731.339 59.003 1.000 28.58 ANISOU 387 C LYS 48 3373 3344 4144 -354 129 -2041 ATOM 388 0 LYS 48 -2.310 30.694 59.396 1.000 27.04 ANISOU 388 0 LYS 48 3849 2793 3633 312 419 -634 MOTA 389 CB LYS 48 1.035 30.654 59.149 1.000 28.95 ANISOU 389 CB LYS 48 3507 3294 4200 -274 - 257 - 738MOTA 390 CG LYS 48 0.775 29.694 60.313 1.000 32.96 ANISOU 390 CG LYS 48 4412 3214 4897 113 -543 - 156 391 MOTA CD LYS 48 1.418 30.222 61.570 1.000 39.92 ANISOU 391 CDLYS 48 5828 4616 4724 705 -1278 - 39MOTA 392 CE LYS 1.217 48 29.320 62.769 1.000 33.67 ANISOU 392 CE LYS 48 3973 4020 4799 1402 -205 - 356 ATOM 393 NZLYS 48 0.731 30.100 63.946 1.000 38.33 ANISOU 393 ΝZ LYS 48 4516 5230 4816 916 -1039 -1555 ATOM 394 ASP N 49 -1.25332.656 59.255 1.000 23.78 ANISOU 394 ASP Ν 49 2796 3136 3104 79 -459 -1588 MOTA 395 CAASP 49 -2.298 33.326 60.006 1.000 24.05 ANISOU 395 CAASP 49 2826 2913 3398 -291 366 -1043 MOTA 396 C ASP 49 -3.67933.181 59.366 1.000 24.45 ANISOU 396 C ASP 49 2721 3270 3300 -220 555 -1454 ATOM 397 ASP 49 -4.63732.951 60.082 1.000 27.10

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                    ASP 49 2863
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   ATOM
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   ATOM
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                              3717 4549
   ATOM
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  ATOM
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51 -5.293 29.580 57.118 1.000 19.40
                   VAL
 ATOM 411 CA VAL
ANISOU 411 CA VAL
                            2631 2056 2683 -12 173 -
-5.631 29.135 58.533 1.000 25.25
 ATOM 412 C
ANISOU 412 C
                   VAL
                                                              173 - 303
                        51
                   VAL
                        51 4453
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 MOTA
                                               2485 -753 587 -955
         413 O VAL
                        51 -6.652 28.454 58.725 1.000 25.07
 ANISOU 413 O VAL
                       51 -6.652 28.454 58.725 1.000 25.07

51 4555 2176 2795 -484 1185 -8

51 -4.377 28.589 56.396 1.000 18.78

51 2729 1786 2620 -72 171 -:

51 3002 1841 2918 295 -13 -4

51 -5.147 27.306 56.021 1.000 24.10

3708 -511 355 6
                                               2795 -484 1185 -827
 ATOM
         414 CB VAL
 ANISOU 414
             CB VAL
 ATOM
         415
             CG1 VAL
                                                            171 - 313
 ANISOU 415
              CG1 VAL
 ATOM
        416
                                                           -13 -480
              CG2 VAL
 ANISOU 416
                       51 3112 2337 3708 -511 355 -
52 -4.836 29.500 59.534 1.000 25.23
              CG2 VAL
                                              3708 -511 355 -846
ATOM
        417
              N ILE
ANISOU 417
                       52 4514 2471 2603 388 76 -87
52 -5.205 29.114 60.921 1.000 24.38
              N
                  ILE
             CA ILE
ATOM
        418
                                                             76 -874
ANISOU 418
ATOM
                           -6.498 29.771 61.355 1.000 24.20
        419
             С
                  ILE
                       52
                                                             19 - 509
ANISOU 419
             С
                  ILE
                        52
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ATOM
                                              3687 -354 114 -648
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                           -7.328 29.182 62.071 1.000 27.73
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                        52
ANISOU 420
             0
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                                              3989 -198 614 -334
ATOM
        421
             CВ
                 ILE
                            -4.016 29.427
                        52
                                              61.829 1.000 27.59
ANISOU 421
             CB ILE
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ATOM
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                                                    590 0 -785
        422
             CG1 ILE
                        52
                            -2.853 28.439
ANISOU 422
                                             61.510 1.000 31.45
             CG1 ILE
                        52
                           3278
                                     5248
                                             3425 741 363 -1288
63.317 1.000 33.62
ATOM
        423
             CG2 ILE
                           -4.293 29.312
                        52
ANISOU 423
             CG2 ILE
                        52
                           3827
                                     6199
        424
                                             2750 881 150 -1454
62.710 1.000 36.22
             CD1 ILE
                           -1.930 28.351
                        52
ANISOU 424
             CD1 ILE
                       52
                            3956
                                     5082
ATOM
                                              4722 979 -601 -234
        425
             N
                 ASP
                       53
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ANISOU 425
                                              60.913 1.000 24.56
             N
                 ASP
                       53
                           3479
                                     2878
ATOM
        426
                                              2974
             CA ASP
                                                      165
                                                           609 - 426
                       53
                           -8.051
ANISOU 426
                                     31.646
                                             61.278 1.000 23.50
            CA ASP
                       53
                           3242
                                     2942
ATOM
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       427
             С
                                                    -5 355 -677
                 ASP
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                                    30.929 60.594 1.000 26.34
                           -9.201
ANISOU 427
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                 ASP
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- 27 -ATOM 428 ASP 0 5 3 -10.342 30.836 61.051 1.000 29.73 ANISOU 428 0 ASP 5 3 3468 3085 3468 3085 4743 -436 937 -1 -7.964 33.084 60.772 1.000 33.83 4743 -436 937 -1142 429 CB ASP 53 ANISOU 429 CB ASP 53 3800 2322 6730 -92 1806 - 933 CG ASP ATOM 430 53 -9.308 33.758 60.583 1.000 32.05 CG ASP ANISOU 430 53 4652 2412 5113 172 -302 -1138 ATOM OD1 ASP 431 53 -9.653 34.524 61.486 1.000 43.68 ANISOU 431 OD1 ASP 53 3661 4686 8248 150 1379 - 3120 ATOM 432 OD2 ASP 53 -9.950 33.556 59.532 1.000 51.30 ANISOU 432 OD2 ASP 53 8386 5033 -2062 -1738 922 6074 MOTA 433 N PHE 54 30.376 59.413 1.000 25.39 -8.933 ANISOU 433 N PHE 54 3372 2640 3637 72.71 -1176 ATOM 434 CA PHE 54 -9.917 29.557 58.704 1.000 24.10 ANISOU 434 CA PHE 54 3015 3264 2876 -366 263 -539 ATOM 435 С PHE 54 -10.180 28.259 59.456 1.000 24.00 ANISOU 435 С PHE 3264 54 3174 2680 -365 459 -688 ATOM 436 O PHE -11.333 27.893 59.686 1.000 28.19 54 ANISOU 436 \circ PHE 54 3551 CB PHE 3246 3914 -549 1305 -1130 54 -9.465 29.273 57.263 1.000 23.62 ATOM 437 ANISOU 437 54 3241 2955 2779 -249 218 -434 CG PHE CG PHE CD1 PHE 54 -10.522 28.499 56.461 1.000 27.62 MOTA 438 ANISOU 438 5 4 4712 2945 2838 -694 -636 1 4 ATOM 439 54 -11.729 29.078 56.087 1.000 31.38 ANISOU 439 CD1 PHE 54 3613 4658 3654 -951 -262 -621 ATOM 440 CD2 PHE 54 -10.283 27.210 56.033 1.000 30.92 ANISOU 440 CD2 PHE 54 5782 5782 3589 2377 -831 293 -844 -12.653 28.406 55.307 1.000 44.29 ATOM 441 CE1 PHE 54 ANISOU 441 CE1 PHE 54 3 5504 5404 5919 -3066 -2057 1178 ATOM 442 CE2 PHE 54 -11.228 26.503 55.306 1.000 38.69 ANISOU 442 CE2 PHE 54 7997 4412 2289 -2803 155 - 387 ATOM 443 CZ PHE 54 -12.424 27.092 54.927 1.000 42.33 ANISOU 443 CZPHE 54 5992 6305 3787 -4256 54 -446 444N PHE 55 -9.126 27.558 59.870 1.000 25.87 ANISOU 444 N PHE 55 3787 2768 3276 -85 431 -839 ATOM 445 CA PHE 55 -9.195 26.310 60.625 1.000 25.69 ANISOU 445 CA PHE 55 3567 3042 3151 68 763 - 711 ATOM 446 С PHE 55 -9.929 26.484 61.944 1.000 27.69 ANISOU 446 С PHE 55 3357 3961 3205 181 703 - 719 ATOM 447 0 -10.745 25.670 62.373 1.000 30.08 PHE 55 ANISOU 447 0 PHE 55 4046 4165 3217 142 878 -127 ATOM 448 CB PHE 55 -7.759 25.873 60.932 1.000 25.48 ANISOU 448 CB PHE 55 3556 3159 2964 117 835 -638 ATOM 449 CG PHE 55 -7.019 25.242 59.762 1.000 26.31 ANISOU 449 CG PHE 55 3437 3039 3522 -468 1068 -1156 ATOM 450 CD1 PHE 55 -7.611 24.820 58.590 1.000 27.09 ANISOU 450 CD1 PHE 55 3553 3895 2845 -1018 1404 - 658 ATOM 451 CD2 PHE 55 -5.651 25.031 59.935 1.000 31.68 ANISOU 451 CD2 PHE 55 3244 4185 4609 -726 1123 - 2221 ATOM 452 CE1 PHE 5 5 -6.878 24.150 57.621 1.000 23.89 ANISOU 452 CE1 PHE 55 3472 2525 3079 -58 551 - 547 MOTA 453 CE2 PHE 5 5 -4.904 24.433 58.950 1.000 31.74 ANISOU 453 CE2 PHE 5 5 3487 4387 4186 226 337 -2304 MOTA 454 CZPHE 55 -5.514 24.004 57.770 1.000 24.23 ANISOU 454 CZPHE 55 3706 2187 3312 414 -22 ATOM 455 Ν GLU 56 27.581 62.629 1.000 30.39 -9.633 ANISOU 455 Ν GLU 56 3961 5033 2553 -308 520 -1110 MOTA 456 CAGLU 56 -10.222 27.875 63.925 1.000 30.18 ANISOU 456 CAGLU

4504

4124

2805

4280 -535

-11.650 28.401 63.820 1.000 33.50

56 -12.470 28.149 64.708 1.000 44.44

-734

1221 - 637

1489 - 892

56

56

56

GLU

GLU

GLU

ATOM

ATOM

ANISOU 457

457

458

С

С

0

4160

4324

PCT/GB98/03860 - 28 -ANISOU 458 O GLU 56 3864 ATOM 459 CB GLU 56 -9.40 56 3864 8872 4150 93 1013 1011 56 -9.403 28.978 64.615 1.000 35.85 ANISOU 459 CB GLU 56 5037 5109 3475 -221 574 -1821 56 -8.192 28.508 65.401 1.000 38.63 ATOM 460 CG GLU ANISOU 460 CG GLU 56 4804 7152 2721 -337 763 -1692 56 -7.395 29.699 65.916 1.000 45.55 ANISOU 474 N GLY 58 4402 3186 4594 5 1572 -1525
ANISOU 475 CA GLY 58 -14.290 28.731
ATOM 476 C GLY 58 4508 4402
ANISOU 476 C GLY 58 -15.449 27.859
ANISOU 476 C GLY 58 -15.449 27.859
ANISOU 477 O GLY 58 -15.245 26.952
ATOM 477 O GLY 58 -15.245 26.952
ANISOU 478 N SER 59 -16.632 28.152
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ANISOU 479 CA SER 59 -17.823 27.359
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ANISOU 479 CA SER 59 -17.763 26.034
ANISOU 480 C SER 59 -17.763 26.034
ANISOU 481 O SER 59 3654
ANISOU 481 O SER 59 3654
ANISOU 481 O SER 59 3027 3655
ATOM 482 CB SER 59 -19.077 28.136
ATOM 483 OG SER 59 3027 3655
ANISOU 483 OG SER 59 3930 5925
ANISOU 484 N GLU 60 -18.589 25.065
ANISOU 484 N GLU 60 -18.589 25.065
ANISOU 485 CA GLU 60 3381 4798
ANISOU 486 C GLU 60 -18.589 3711
ANISOU 486 C GLU 60 -19.033 24.055
ANISOU 487 O GLU 60 -18.616 23.437 56.361 1.000 29.91 60 -18.616 23.437 56.361 1.000 29.91 1378 - 847 ANISOU 487 60 3708 3040 GLU

4615 -679 2037 -604

-1599 748 -1000

60 -19.390 22.742 59.488 1.000 38.26

3958

488 CB GLU

ANISOU 488 CB GLU 60 5012 5567

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CG GLU 60 -18.625 22.182 60.678 1.000 42.01
CG GLU 60 5470 5439 5055 503 950 -782
CD GLU 60 -17.307 21.528 60.312 1.000 45.34
           489
 ANISCU 489 CG GLU
                               60
60
 ATOM
           490 CD GLU
 ANISOU 490 CD GLU
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-17.219 20.867 59.264 1.000 49.69
 ATOM
           491
                  OE1 GLU
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60 -16.323 21.659 61.084 1.000 43.62
 ANISOU 491
                  OE1 GLU
 ATOM
           492
                  OE2 GLU
ATOM 492 0E2 GLU 60 4677 4974 6924 -1984 109 -
ATOM 493 N ALA 61 -19.928 25.028 57.167 1.000 34.26
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 ANISOU 493 N
           493 N ALA 61 3091 3912 6014 -81 1209 -1122
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 ATOM
ATOM 494 CA ALA 61 -20.408 25.324 55.823 1.000 33.07

ANISOU 494 CA ALA 61 1647 4409 6508 -228 657 -1

ATOM 495 C ALA 61 -19.314 25.876 54.938 1.000 30.69

ANISOU 495 C ALA 61 2053 3742 5866 -59 640 -1

ATOM 496 O ALA 61 -19.138 25.482 53.790 1.000 31.15

ANISOU 496 O ALA 61 2754 2893 6189 31 793 -1285

ATOM 497 CB ALA 61 -21.543 26.336 55.932 1.000 34.43

ANISOU 497 CB ALA 61 2783 4403 5897 288 1210 -1

ATOM 498 N GLU 62 -18.568 26.824 55.498 1.000 28.80

ANISOU 498 N GLU 62 2168 3404 5371 -9 915 -964

ATOM 499 CA GLU 62 -17.478 27.395 54.704 1.000 26.78
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                                                             5866 -59 640 -1066
                                                                        31 793 -1285
                                                                                 1210 - 1650
ANISOU 498 N GLU 62 2168 3404 5371 -9 915 -9 64
ATOM 499 CA GLU 62 -17.478 27.395 54.704 1.000 26.78
ANISOU 499 CA GLU 62 2339 2374 5461 423 871 -413
ATOM 500 C GLU 62 -16.432 26.330 54.389 1.000 22.61
ANISOU 500 C GLU 62 2569 1621 4402 84 1049 -376
ATOM 501 O GLU 62 -15.851 26.316 53.289 1.000 24.41
ANISOU 501 O GLU 62 2399 2669 4209 -132 801 -548
ANISOU 502 CB GLU 62 -16.861 28.591 55.429 1.000 32.86
ANISOU 503 CG GLU 62 -17.739 29.834 55.554 1.000 34.69
ANISOU 503 CG GLU 62 2824 2859 7499 916 -95 -1439
                                                                       251 2039 - 1358
ANISOU 503 CG GLU
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                                                                              -95 -1430
           504 CD GLU
ATOM
                               62
ANISOU 504
                 CD GLU
                               62
                                     4998
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          505 OE1 GLU 62
ATOM
ANISOU 505 OE1 GLU 62
                                    4844
                                                 3636
                                                             7068
                                                                      1268 34 - 1673
        506 OE2 GLU 62
ATOM
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ANISOU 506 OE2 GLU 62
                                     7600 2889 6658 -525 1698 -
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                                    7600
                                                                       -525 1698 -1099
ATOM
         507 N LYS 63
ANISOU 507 N
                       LYS 63
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                                                 2380
                                                             4723
                                                                       312 1050 8
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ATOM
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ANISOU 508 CA LYS 63
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                                                 2894
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ANISOU 509 C LYS
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2930 3038 2540 24.423 21.7
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ATOM
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ANISOU 510 O LYS
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           511
ATOM
                 CB LYS
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                               63
ANISOU 511
                 CB LYS 63
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                                    3411
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ATOM
           512
                 CG LYS 63
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ANISOU 512
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ATOM
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ANISOU 513
                 CD LYS 63 3132
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                 CE LYS 63 -12.761 24.695 59.560 1.000 28.96
CE LYS 63 4342 3579 3083 -317 -286 -
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ATOM
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ANISOU 514
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MOTA
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ANISOU 515
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MOTA
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ANISOU 518 C
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    ATOM
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    ANISOU 524
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                NH1 ARG
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    ANISOU 525
                NH1 ARG
                         64
    ATOM
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                NH2 ARG
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   ATOM
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                        65
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                  VAL
  ATOM
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                                                         79 - 487
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  ATOM
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 ATOM
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              CG2 VAL
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 ANISOU 538
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              CG2 VAL
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 ATOM
         539
             Ν
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                 THR
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2202 2014 2827 192 224 -
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 ATOM
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ATOM
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ATOM
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ANISOU 548
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ANISOU 549
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WO 99/33994 PCT/GB98/03860 - 31 -ATOM 550 CB SER 68 -11.958 17.303 47.257 1.000 17.84 1459 2139 3182 -87 647 -313 ANISOU 550 CB SER 68 MOTA 551 OG -10.998 18.259 46.904 1.000 17.21 SER 68 ANISOU 551 OG SER 68 1659 1987 2893 -75 364 - 49ATOM 552 N PRO 69 -14.929 16.284 47.054 1.000 15.89 1574 1661 2803 -201 -103 -280 -15.877 15.182 47.339 1.000 16.42 ANISOU 552 N PRO 69 ATOM 553 PRO CA69 PRO ANISOU 553 CA69 ATOM 554 С PRO 69 ANISOU 554 С 1633 1578 3331 -199 266 -424 -15.794 12.997 48.287 1.000 18.35 PRO 69 ATOM 555 0 PRO 69 ANISOU 555 0 PRO 69 ATOM 556 CB PRO 69 ANISOU 556 CB PRO 1354 2279 2733 -360 155 -729 -15.799 15.637 45.008 1.000 16.72 69 ATOM 557 CG PRO 69 ANISOU 557 1553 1971 2827 -359 38 -452 -15.059 16.797 45.631 1.000 17.10 1553 1971 CG PRO 69 MOTA 558 CD PRO 69 ANISOU 558 CD PRO 69 1918 1804 2776 -344 -119 -313 -13.884 13.746 47.366 1.000 18.07 ATOM 559 N VAL 70 ANISOU 559 N VAL 70 1716 1764 3384 -89 292 - 215 ATOM 560 CA VAL 70 -13.100 12.594 47.824 1.000 17.34 ANISOU 560 CA VAL 70 1763 1851 2974 -20 260 - 196 ATOM 561 С VAL -11.995 13.142 48.720 1.000 17.59 70 ANISOU 561 С VAL 70 2207 1686 2788 -180 159 -142 MOTA 562 0 VAL 70 -11.431 14.186 48.389 1.000 18.59 ANISOU 562 0 VAL 70 1794 1688 3581 -4 9 1 5 2 MOTA 563 CВ VAL 70 -12.429 11.757 46.724 1.000 18.10 1922 1756 ANISOU 563 CВ VAL 70 3199 -353 560 -446 564 CG1 VAL ATOM 70 -13.441 10.754 46.213 1.000 20.54 ANISOU 564 CG1 VAL 70 1927 2611 3268 -369 76 ~663 ATOM 565 CG2 VAL 70

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- 32 -ANISOU 580 N MET 73 2057 1748 2951 -58 -254 - 426 ATOM 581 CAMET 73 16.117 -5.867 50.394 1.000 16.58 ANISOU 581 C.A. MET 73 1796 1708 2797 88 - 302 - 340 ATOM 582 C MET 73 16.618 -5.07349.198 1.000 16.65 ANISOU 582 С MET 73 1514 1787 3027 241 -162 - 420 MOTA 583 0 MET 73 -3.91117.039 49.292 1.000 19.39 ANISOU 583 0 1705 MET 73 2313 3348 -112 -240 -540 MOTA 584 CВ MET 73 -4.925 51.469 1.000 20.56 15.531 ANISOU 584 CВ MET 73 2099 2629 3083 345 -507 - 286 MOTA 585 CG MET 73 -5.703 15.154 52.715 1.000 30.33 ANISOU 585 CG MET 73 3008 5133 -69 -609 1 0 2 7 3384 ATOM 586 SD MET 73 -4.692 14.263 53.891 1.000 36.13 ANISOU 586 SD MET 73 4121 5050 4558 336 -918 1596 ATOM 587 CE MET 73 -3.165 13.987 53.082 1.000 58.07 ANISOU 587 CE MET 73 2810 8820 10435 975 -1592 -3138 ATOM 588 N ARG 74 -5.687 16.632 48.025 1.000 16.83 ANISOU 588 N ARG 74 1699 2982 -6 -211 1 3 1 46.817 1.000 15.87 1714 ATOM 589 CAARG 74 -5.099 17.215 ANISOU 589 CAARG 74 1365 1618 3046 -17 52 - 325 ATOM 590 C ARG 74 -5.359 18.714 46.761 1.000 14.22 ANISOU 590 С ARG 74 1484 1651 2269 141 -32 - 42MOTA 591 0 ARG 74 -4.47219.488 46.353 1.000 15.45 ANISOU 591 0 ARG 74 1525 1758 2586 -12 -46 - 73ATOM 592 CB ARG 74 -5.675 16.530 45.566 1.000 15.68 ANISOU 592 CB ARG 74 1330 1667 2959 160 -14 - 311ATOM 593 CG ARG 74 -4.890 16.941 44.299 1.000 16.46 ANISOU 593 CG ARG 74 1325 1870 3059 -175 55 - 395 MOTA 594 CD ARG 74 = -5.655 16.396 43.072 1.000 16.37 ANISOU 594 CDARG 74 1789 1533 2899 -181 -8 -177 ATOM 595 ΝE ARG 74 -4.84016.601 41.857 1.000 19.21 ANISOU 595 ΝE ARG 74 2289 1990 3020 -142 241 -156 ATOM 596 CZARG 74 -4.944 17.626 41.039 1.000 17.00 ANISOU 596 CZ ARG 74 1545 2351 2562 -67 26 - 147ATOM 597 NH1 ARG 74 18.573 41.213 1.000 18.00 -5.878 ANISOU 597 NH1 ARG 74 1818 2383 2638 51 -66 - 220 ATOM 598 NH2 ARG 74 -4.144 17.703 39.987 1.000 20.50 ANISOU 598 NH2 ARG 2285 74 2972 2532 -110 310 -387 ATOM 599 Ν ARG 75 -6.579 19.151 47.101 1.000 15.28 ANISOU 599 Ν ARG 75 1755 1544 2507 137 340 - 173ATOM 600 CAARG 75 -6.999 20.550 46.980 1.000 14.68 ANISOU 600 CA ARG 75 1679 1627 2272 236 98 - 150 ATOM 601 C ARG 75 20.869 48.122 1.000 14.75 -7.956 ANISOU 601 C 75 ARG 1445 1747 2414 124 133 - 233 ATOM 602 0 ARG 75 -8.760 19.989 48.460 1.000 18.12 ANISOU 602 0 75 ARG 1677 2109 3101 -156 458 -433 MOTA 603 CB ARG 75 -7.747 20.804 45.668 1.000 15.59 ANISOU 603 CB ARG 75 1577 2030 2317 · 1 46 - 106 ATOM 604 CG ARG 75 -6.848 20.634 44.441 1.000 15.63 ANISOU 604 CG ARG 75 1495 2334 9 147 2 2 0 2110 ATOM 605 CDARG 75 -5.712 21.618 44.334 1.000 15.59 ANISOU 605 CDARG 75 1658 1792 2475 11 130 - 10 ATOM 606 NΕ ARG 75 -5.061 21.601 43.011 1.000 15.25 ANISOU 606 NΞ ARG 75 1421 1779 2596 122 227 144 MOTA 607 CZARG 75 -3.957 20.865 42.732 1.000 14.90 ANISOU 607 CZARG 75 1079 2361 2221 71 -86 2 4 2 ATOM 608 NH1 ARG 75 20.091 43.664 1.000 16.18 -3.405 ANISOU 608 NH1 ARG 75 1804 1722 2623 -134 -387 3 3 7 ATOM 609 NH2 ARG 75 -3.418 20.940 41.518 1.000 15.83 ANISOU 609 NH2 ARG 75 1677 2107 2232 -193 221 0 ATOM 610 N GLY 76 22.086 48.651 1.000 16.06 -7.895 ANISOU 610 N GLY 76 1686 1904 2513 109 220 - 464

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MOTA
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                     101 2042
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            CD2 TYR
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- 35 -MOTA 672 101 -7.406 25.796 51.036 1.000 19.63 CE1 TYR 101 1977 ANISOU 672 CE1 TYR 1776 3704 88 -241 - 221 ATOM 673 CE2 TYR 101 -5.147 101 2060 26.386 50.478 1.000 20.46 ANISOU 673 CE2 TYR 2608 3108 239 674 CZ TYR 101 -6.504 26.392 50.166 1.000 20.29 ANISOU 674 CZTYR 101 2187 2397 3127 -73 101 -6.932 26.995 49.000 1.000 23.34 -353 - 260 675 OH TYR 101 2790 ANISOU 675 OH TYR 2555 3523 -3 -641 5 2 MOTA 676 N SER ANISOU 676 N SER 102 1618 1890 2041 -61 -109 - 477 21.792 49.980 1.000 14.52 ATOM 677 CA SER 102 -3.797 102 1684 ANISOU 677 CA SER 2030 -108 62 -276 1802 22.670 48.747 1.000 14.99 ATOM 678 C 102 -4.011 SER ANISOU 678 C SER 102 1545 1790 2361 -296 -41 2 1 679 ATOM 102 -5.167 0 SER 23.105 48.477 1.000 16.73 102 1589 2342 2425 2 128 - 3 102 -4.163 20.340 49.593 1.000 13.82 ANISOU 679 0 SER ATOM 680 CB SER ANISOU 680 CB SER 102 1692 1548 2013 174 9 -138 MOTA 681 OG SER 102 -3.996 19.476 50.720 1.000 16.06 OG SER ANISOU 681
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- 37 -ATOM 733 O PHE 110 -12.433 29.948 48.494 1.000 24.64 733 O PHE 110 2051 2461 4851 612 328 -ANISOU 733 O PHE 110 2051 2461 4851 612 328 -779 110 -9.607 30.243 47.520 1.000 19.92 734 CB PHE CB PHE ANISOU 734 735 CG PHE ANISOU 735 CG PHE 110 2009 2209 3179 -321 327 -791 110 -7.177 29.680 47.287 1.000 20.59 736 CD1 PHE 110 2071 2080 3674 -274 236 -331 110 -8.437 30.035 45.299 1.000 20.19 110 2557 1914 3200 112 543 -289 110 -6.034 29.454 46.559 1.000 21.06 ANISOU 736 CD1 PHE ATOM 737 CD2 PHE ANISOU 737 CD2 PHE MOTA 738 CE1 PHE 738 CEI PHE 110 -0.034 29.434 40.539 1.000 21.06
738 CEI PHE 110 2020 2309 3673 -386 165 -622
739 CE2 PHE 110 -7.277 29.811 44.547 1.000 20.77
740 CZ PHE 110 2495 2138 3257 197 504 -398
0U 740 CZ PHE 110 -6.081 29.518 45.175 1.000 22.42
0U 740 CZ PHE 110 2747 2092 3678 531 339 -357 ANISOU 738 CE1 PHE ATOM ANISOU 739 ATOM ATOM 740 CZ PHE 110 -6.081 29.518 45.175 1.000 22.42

ANISOU 740 CZ PHE 110 2747 2092 3678 531 339 -357

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ANISOU 741 N PRO 111 2250 2153 3996 -72 871 -620

ATOM 742 CA PRO 111 3895 2210 4621 698 1514 -671

ANISOU 743 C PRO 111 -12.287 30.389 51.195 1.000 28.23

ATOM 743 C PRO 111 -12.333 31.866 50.784 1.000 30.57

ANISOU 744 O PRO 111 4528 2026 5061 410 410 -1041

ANISOU 744 O PRO 111 -11.390 32.340 50.115 1.000 31.71

ANISOU 745 CB PRO 111 4040 2236 5774 -179 -597 - 12

ATOM 746 CG PRO 111 5609 2702 4303 671 1671 -790

ATOM 746 CG PRO 111 -10.646 29.326 52.627 1.000 33.20

ATOM 746 CG PRO 111 2742 3316 3835 -931 1324 -192

ANISOU 747 CD PRO 111 2742 3316 3835 -931 1324 -192

ANISOU 747 CD PRO 111 2587 2307 3522 -471 541 -623

ANISOU 748 N SER 112 -13.337 32.641 51.150 1.000 42.13

ANISOU 749 CA SER 112 -13.368 34.026 50.672 1.000 44.05

ANISOU 749 CA SER 112 6799 2255 7684 1107 -485 -826 ANISOU 740 CZ PHE 110 2747 ANISOU 749 CA SER 112 6799 2255 7684 1107 -485 -826 112 -13.262 34.157 49.149 1.000 68.28 ATOM 750 C SER 750 C SER 112 13632 4498 7812 -1855 -2077 1301 751 O SER 112 -12.347 34.825 48.646 1.000 95.18 ANISOU 750 C SER ATOM ANISOU 751 O SER 112 15991 11425 8747 -4337 -70 1985 ATOM 752 CB SER 112 -12.493 35.069 51.349 1.000 39.31 ANISOU 752 CB SER 112 2247 4535 8153 580 1662 -1437 ATOM 753 OG SER 112 -11.474 34.624 52.213 1.000 37.49 ATOM 753 OG SER 112 -11.474 34.624 52.213 1.000 37.49

ANISOU 753 OG SER 112 7213 2453 4579 806 747 -1152

ATOM 754 N ASP 114 -9.515 37.322 49.945 1.000 36.40

ATOM 755 CA ASP 114 3476 2118 8237 1254 403 1484

ATOM 755 CA ASP 114 -8.205 37.586 50.600 1.000 30.79

ATOM 756 C ASP 114 3503 2856 5340 1229 1240 9 9 6

ANISOU 756 C ASP 114 -7.242 36.402 50.648 1.000 26.16

ATOM 757 O ASP 114 -6.031 36.458 50.338 1.000 25.45

ANISOU 757 O ASP 114 -6.031 36.458 50.338 1.000 25.45

ATOM 758 CB ASP 114 -8.595 37.874 52.075 1.000 43.68

ANISOU 759 CG ASP 114 -7.391 38.386 52.835 1.000 46.96

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ANISOU 760 OD1 ASP 114 -6.487 38.959 52.189 1.000 83.49

ANISOU 760 OD1 ASP 114 13724 9866 8132 -6354 650 -3056 OD1 ASP 114 13724 9866 8132 -6354 650 -3056 OD2 ASP 114 -7.370 38.262 54.071 1.000113.59 761 ANISOU 761 OD2 ASP 114 27880 10550 4730 -6984 -159 - 2575 115 -7.831 35.323 51.153 1.000 22.32 762 N PHE ANISOU 762 N PHE 115 2620 2062 3799 204 954 - 114 ATOM 763 CA PHE 115 -7.115 34.026 51.183 1.000 22.69

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ANISOU 76	2		- 38 -	
	• •	HE 115 2765	1909	2047
ATOM 764 ANISOU 764		HE 115 -6.5	02 33 754	
		HE 115 2146	2316	
	9 O Pi	HE 115 -5.3	28 33.362	
ANISOU 769		E 115 2153	2011	49.758 1.000 20.51
ATOM 766		IE 115 -8.0		304/ 323 488 150
ANISOU 766	CB PH			51.638 1.000 20.76
ATOM 767	CG P#		1946	22/4 -3 563 - 472
ANISOU 767		[E 115 2360		51.998 1.000 20 23
ATOM 768	בים ומי	E 115 -6.9	1854	3403 -155 62G 377
ANISOU 768	CD1 PH	E 115 2572		51.041 1.000 20 35
ATOM 769	CD2 PH	E 115 -7.4	1786	33/2 -195 110 756
ANISOU 769	CD2 PH	E 115 2802		53.309 1 000 21 11
ATOM 770	CF1 DH	E 115 -6.35	1932	348/ -113 17 600
ANISOU 770	CE1 PH	E 115 2502		51.325 1.000 21 00
ATOM 771	CE2 PH		1728	2/04 -295 /71
ANISOU 771	CE2 PH			53.623 1.000 27 40
ATOM 772	CZ PH		1955	3/45 444 43 - 572
ANISOU 772	CZ PH			52.655 1.000 24.92
ATOM 773	N GL		1889	4222 50 1519 2 2 1
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ATOM 774	CA GLU		1835	3990 339 261
ANISOU 774	CA GLU	0./3		3790 338 261 - 13 47.444 1.000 20.90
ATOM 775	C GLU		1965	3742 224 74 1 1 6
ANISOU 775	C GLU			45 / = 1 1 0
ATOM 776	O GLU		1899	
ANISOU 776	O GLU			3845 439 -108 4 4 8 46.604 1.000 20.18
ATOM 777	CB GLU		2147	3312 424 73 1 3 9
ANISOU 777	CB GLU			46.385 1.000 24.22
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ANISOU 778	CG GLU	,		4139 -467 -237 5 1 9 44.980 1.000 23.27
ATOM 779	CD GLU	2 2 2 3	2465	
ANISOU 779	CD GLU			43.910 1.000 25.02
ATOM 780	OE1 GLU		2703	4107 -510 -739 1509
ANISOU 780	OE1 GLU		33.306	44.207 1.000 34.83
ATOM 781	OE2 GLU		± 0 0 0	6161 -203 -928 1566
ANISOU 781	OE2 GLU		33.030	42.763 1.000 40.92
ATOM 782	N ARG		1 4 / 4	3988 -24 -968 6 9 3
3 3TT 0 0	N ARG	117 -5.549	35.571	47.300 1.000 20.60
ATOM 783	CA ARG	117 2299	+ U + 1	3718 382 -10 469
ANISOU 783	CA ARG	117 -4.374	36.374	46.866 1.000 22 65
ATOM 784	C ARG	117 2230	1 / J 1	4086 351 107 1 = 5
ANISOU 784	C ARG	117 -3.163 117 2269	35.911 .	47.648 1.000 21.87
ATOM 785	O ARG		~000	4178 252 179 9 7
ANISOU 785	O ARG	117 -2.060 117 2197	35.789	47.102 1.000 22.10
ATOM 786	CB ARG	117 4 500	2270	3931 216 41 205
ANISOU 786	CB ARG	117 -4.682 117 2849	37.861	47.105 1.000 29 47
ATOM 787	CG ARG	117 2 405		6658 259 -555 - 1
ANISOU 787	CG ARG	117 -3.485 117 3905	38.815	47.046 1.000 40 24
ATOM 788 (CD ARG	117 -3.745	2307	3818 -819 -1330 476
ANISOU 788 (CD ARG	117 4698	40.160 4	17.716 1.000 52 75
ATOM 789 7	VE ARG	117 2 22	2040	14496 - 595 - 1653 - 1660
ANISOU 789 1	NE ARG	117 -3.934	39.987 4	19.155 1.000 68 00
ATOM 790 (ZZ ARG	117 8247	3/13 1	$\frac{12872}{1842} = \frac{3441}{1842}$
ANISOU 790 d	Z ARG	117 -3.166	40.448 5	0.126 1.000 78.38
ATOM 791 N	VH1 ARG	117 13026	2020 [.1097 283 448 - 2400
ANISOU 791 N	JH1 ARG	117 -2.097	41.186 4	9.849 1.000 89 01
ATOM 792 N	H2 ARG	117 14218	11488 g	115 -3550 -6761 3577
ANISOU 792 N	IH2 ARG	117 -3.479	40.189 5	1.391 1.000 82.58
ATOM 793 N	ILE	117 16575	2856 1	1947 2617 2551 - 2095
ANISOU 793 N		118 -3.334	35.759 4	8.954 1.000 21.70
		118 2319	1 7 0 7	
			-	12/ 311 271 - 314

- 39 -ATOM 794 CA ILE 118 -2.206 35.425 49.810 1.000 20.99 ANISOU 794 CA ILE 118 2546 1624 3805 408 294 - 470795 C ATOM ILE 118 -1.596 34.073 49.475 1.000 18.79 ANISOU 795 С ILE 118 2222 1534 3384 573 - 201 218 ATOM 796 O ILE 118 -0.409 33.858 49.323 1.000 17.27 O ILE ANISOU 796 118 2194 1663 2707 283 351 - 136 797 ATOM 118 -2.588 35.542 51.293 1.000 22.62 ANISOU 797 CB ILE 118 2702 1997 3895 276 416 -856 MOTA 798 CG1 ILE 118 -2.916 36.995 51.700 1.000 27.54 ANISOU 798 CG1 ILE 118 5077 1801 3587 503 768 - 401MOTA 799 CG2 ILE 118 -1.552 34.940 52.206 1.000 23.59 ANISOU 799 CG2 ILE 118 3084 2274 3606 183 254 -818 CD1 ILE MOTA 800 118 -3.493 37.115 53.096 1.000 29.35 ANISOU 800 CD1 ILE 118 5212 2054 3885 558· 1114 - 645 MOTA 801 Ν TRP 33.069 49.341 1.000 17.93 119 -2.454 ANISOU 801 Ν TRP 119 2378 . 1605 147 -80 -2.69 2828 CA TRP ATOM 802 119 -2.035 31.688 49.103 1.000 16.57 ANISOU 802 CA TRP 119 2126 1538 2630 152 -25 - 16 ATOM 803 \mathcal{C} TRP 119 -1.575 31.476 47.676 1.000 16.98 ANISOU 803 C TRP 119 2126 1723 2604 269 -91 - 51 ATOM 804 0 TRP 119 -0.700 30.640 47.455 1.000 17.58 ANISOU 804 0 TRP 119 1892 1674 3113 135 181 6 3 805 CB TRP 119 -3.127 30.690 49.591 1.000 18.32 ANISOU 805 CB TRP 119 2156 1789 3014 -34 806 CG TRP 119 -2.934 30.457 51.082 1.000 18.27 ANISOU 806 CG TRP 119 2208 3025 86 349 5 6 1711 807 MOTA CD1 TRP 119 -3.354 31.273 52.103 1.000 20.36 ANISOU 807 CD1 TRP 119 2624 2029 3083 156 276 - 153ATOM 808 29.383 51.683 1.000 18.61 2055 2967 134 263 1 CD2 TRP $119^{3} - 2.213$ ANISOU 808 119 2049 CD2 TRP 263 110 119 -2.955 30.773 53.323 1.000 20.55 ATOM 809 NE1 TRP ANISOU 809 NE1 TRP 119 2471 2229 3109 92 266 - 106 ATOM 810 CE2 TRP 119 -2.260 29.603 53.073 1.000 20.21 ANISOU 810 CE2 TRP 119 2529 2258 2893 180 754 MOTA 811 CE3 TRP 119 -1.576 28.258 51.147 1.000 18.29 ANISOU 811 CE3 TRP 119 2258 1714 2977 42 -70 - 20 ATOM 812 CZ2 TRP 119 -1.636 28.728 53.981 1.000 21.97 ANISOU 812 119 2876 CZ2 TRP 2945 2526 384 51 - 106 119 -0.968 27.375 52.045 1.000 19.35 ATOM 813 CZ3 TRP ANISOU 813 CZ3 TRP 119 2576 2028 2750 187 415 299 CH2 TRP ATOM 814 119 -1.026 27.618 53.442 1.000 21.67 ANISOU 814 119 3033 CH2 TRP 2379 2823 350 250 9 7 MOTA 815 Ν THR 120 -2.129 32.192 46.701 1.000 16.93 ANISOU 815 N THR 120 2023 1833 2577 122 -112 1 8 MOTA 816 CA THR 120 -1.598 32.086 45.342 1.000 17.85 ANISOU 816 CA THR 120 1915 2469 2398 222 -371 - 324ATOM 817 С 120 -0.169 32.587 45.288 1.000 17.15 THR ANISOU 817 С 120 2031 THR 1855 2629 241 -155 1 9 2 818 0 THR 120 0.700 31.960 44.674 1.000 18.67 ANISOU 818 0 THR 120 1996 1887 3212 389 -131 1 7 7 120 -2.487 32.865 44.344 1.000 18.10 MOTE 819 CB THR ANISOU 819 CB THR 120 1951 2204 2720 28 -93 3 4 5 ATOM 820 OG1 THR 120 -3.773 32.238 44.284 1.000 20.49 ANISOU 820 OG1 THR 120 1807 2801 31/9 55-553 32.803 42.933 1.000 22.46 2830 475 118 7 0 5 2801 3179 59 -363 558 MOTA CG2 THR 821 120 -1.919 CG2 THR ANISOU 821 120 2438 ATOM 822 N GLN 121 0.094 33.708 45.956 1.000 18.62 ANISOU 822 N GLN 121 2180 1657 3237 123 -94 213 823 CA GLN 121 1.466 34.232 45.993 1.000 18.15 ANISOU 823 CA GLN 121 2077 1698 3119 77 96 5 2 0 33.284 46.718 1.000 17.04 ATOM 824 121 2.412 GLN

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ANISOU 831 N TYR 122 2389
ATOM 832 CA TYR 122 2.795
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ANISOU 834 O TYR 122 1891
ATOM 835 CB TYR 122 2.795
ATOM 836 CB TYR 122 2.795
ATOM 837 C TYR 122 1891
ANISOU 838 C TYR 122 1891
ANISOU 838 C TYR 122 1891
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ATOM 835 CB TYR 122 2.795
ATOM 835 CB TYR 122 1891
ATOM 835 CB TYR 122 2.795
ATOM 835 CB TYR 122 2.795
ATOM 835 CB TYR 122 1891
ATOM 835 CB TYR 122 2.795
ATOM 836 ATOM 837 CB TYR 122 2.795
ATOM 837 CB TYR 122 2.859
ATOM 838 ATOM 838 CB TYR 122 2.859
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ATOM 837 CB TYR 122 2.859
ATOM 836 ATOM 837 CB TYR 122 2.859
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CD2 TYR
CE1 TYR
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ATOM 855 CA ASP 124 4.060 30.640 43.544 1.000 17.82 ANISOU 855 CA ASP 124 2103 1747 2921 405 -24 314 MOTA 856 C 124 5.490 ASP 30.733 44.024 1.000 17.52 ANISOU 856 C ASP 124 1999 181 94 8 9 1439 3219 ATOM 857 0 ASP 124 6.402 43.317 1.000 17.18 30.324 ANISOU 857 О 124 2086 ASP 1427 3015 34 181 177 ATOM 858 CB AASP 124 3.639 31.997 42.942 0.534 21.77 ANISOU 858 CB AASP 124 3475 2089 2706 642 -372 5 9 7 859 CG AASP 124 4.381 MOTA 41.659 0.534 19.28 32.304 ANISOU 859 CG AASP 124 2376 1982 2967 173 -553 4 9 5 MOTA 860 OD1 AASP 124 4.223 31.538 40.678 0.534 21.03 ANISOU 860 OD1 AASP 124 2189 2636 3164 -28 76 2 1 MOTA 861 OD2 AASP 124 5.068 33.348 41.639 0.534 24.96 ANISOU 861 OD2 AASP 124 3681 2052 3752 -296 -1067 889 ATOM 862 CB BASP 124 3.632 31.975 42.908 0.466 19.67 ANISOU 862 CB BASP 124 2559 1993 2923 1003 673 446 CG BASP 124 2.368 CG BASP 124 3552 MOTA 863 31.849 42.089 0.466 22.78 ANISOU 863 3217 1889 872 177 1175 OD1 BASP 124 2.021 MOTA864 30.781 41.545 0.466 27.78 OD1 BASP 124 2138 ANISOU 864 3932 4483 100 503 347 ATOM 865 OD2 BASP 124 1.703 32.893 41.902 0.466 29.73 OD2 BASP 124 3845 ANISOU 865 3804 3646 1239 -312 1644 ATOM 866 125 5.669 NARG 31.416 45.153 1.000 16.65 125 1942 125 7.038 125 1918 125 7.662 ANISOU 866 1350 Ν ARG 3032 276 139 276 ATOM 867 CA ARG 31.528 45.646 1.000 17.58 CA ARG ANISOU 867 1819 2944 98 177 2 4 1 MOTA 868 C ARG 30.188 45.992 1.000 17.38 125 1544 125 8.841 ANISOU 868 C ARG 1777 3282 -42 40 273 869 0 ARG 29.942 45.754 1.000 18.26 ANISOU 869 O ARG 125 1639 1669 3631 -97 91 - 233870 CB ARG MOTA 125 7.062 32.468 46.851 1.000 20.45 125 2219 ANISOU 870 CB ARG 2162 3387 -244 450 -274 ATOM 871 CG ARG 125 6.860 46.344 1.000 28.23 33.916 ANISOU 871 CG ARG 125 3178 2007 5542 147 666 - 222 ATOM 872 CD ARG 125 6.693 34.891 47.477 1.000 31.76 ANISOU 872 CD ARG 125 3065 2279 6725 -628 1455 - 993 ATOM 873 NE ARG 125 6.496 36.221 46.932 1.000 40.81 ANISOU 873 NE ARG 125 3332 2095 10080 -169 1790 - 694 874 CZ ARG ATOM 125 5.970 37.229 47.628 1.000 43.42 ANISOU 874 CZ ARG 125 4531 2891 9076 839 2072 - 188MOTA 875 NH1 ARG 125 5.551 37.025 48.866 1.000 38.62 ANISOU 875 NH1 ARG 125 3999 2858 7816 -858 61 -700 MOTA 876 NH2 ARG 125 5.858 38.382 47.006 1.000 42.11 ANISOU 876 NH2 ARG 125 5319 2652 8030 908 1627 - 681 ATOM 877 N ${ t GLN}$ 126 6.884 29.282 46.557 1.000 15.28 ANISOU 877 126 1876 N GLN 1527 2404 -70 13 - 60 ATOM 878 CA GLN 126 7.376 27.929 46.853 1.000 15.37 ANISOU 878 CA GLN 126 1726 1625 2488 -54 -31220ATOM 879 С GLN 126 7.649 27.150 45.578 1.000 14.21 ANISOU 879 C GLN 126 1643 1268 2488 -75 -398 7 1 MOTA 880 0 GLN 126 8.682 26.462 45.496 1.000 15.36 ANISOU 880 0 GLN 126 1531 1554 2753 -37 -316 5 3 MOTA 881 СЗ GLN 126 6.356 27.158 47.702 1.000 17.40 ANISOU 881 СЗ GLN 126 2034 1313 3264 158 293 4 3 882 CG GLN 126 6.336 27.634 49.150 1.000 26.14 ANISOU 882 CG GLN126 4503 1690 3739 431 1908 - 732 MOTA 883 CD126 5.208 126 2957 GLN 26.998 49.891 1.000 21.95 ANISOU 883 CD GLN 2670 2713 0 -123 1 0 2 884 OE1 GLN 126 4.051 27.372 49.730 1.000 42.52 ANISOU 884 OE1 GLN 126 2994 5747 7416 -62 -1272 3147 885 NE2 GLN 126 5.524 26.003 50.691 1.000 28.32

- 41 -

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- 42 -
            NE2 GLN 126 2867
 ANISOU 885
                                   3971
                                           3922 -184 -780 1311
        886 N
                      127 6.797
                 TYR
                                  27.287 44.574 1.000 14.52
                      ANISOU 886
            N
                 TYR
                                                -41 -373 - 36
 ATOM
        887
            CA TYR
                                  26.554 43.317 1.000 13.93
 ANISOU 887
            CA TYR
                                                -136 -234 150
 ATOM
       888
            С
                 TYR
                      ANISOU 888
            С
                 TYR
                                           2745 24 -195 190
       889 0
 ATOM
                 TYR
 ANISOU 889
            0
                 TYR
                      127 1611
                                 1580
                                           2277 34 -252 9
                      127 5.801 26.676 42.435 1.000 14.00
        890 CB TYR
890 CB TYR
 ATOM
ANISOU 890
                      127 1510
                                 1549
                                                29 -180 - 70
                                           2258
                      127 5.752 25.795 41.202 1.000 12.33
ATOM
        891
            CG
                TYR
ANISOU 891
            CG TYR
                      127 1315
                                 1037
                                           2334 -34 -187 4 5
        892
MOTA
             CD1 TYR
                      127 6.483 24.626 41.024 1.000 14.05
ANISOU 89.2
             CD1 TYR
                      127 1810
                                 1158
                                          2371
                                                 7 -84 - 8
        893
ATOM
             CD2 TYR
                     127 4.837 26.086 40.206 1.000 15.71
            CD2 TYR
CE1 TYR
ANISOU 893
                      127 1936
                                          2484 55 -513 2 1
                                 1548
ATOM
        894
                      127 6.382 23.829 39.899 1.000 13.10
            CE1 TYR
ANISOU 894
                      127 1450 999 2529 -101 -227 -62
127 4.661 25.322 39.071 1.000 15.07
                      127 1450
            CE2 TYR
ATOM
       895
                     127 4.661 25.322 39.071 1.000 15.07

127 1928 1620 2177 158 -342 19

127 5.440 24.179 38.934 1.000 13.71

127 1617 1348 2245 -146 -106 24

127 5.337 23.386 37.811 1.000 15.04

127 1682 1755 2279 -87 -60 5
ANISOU 895
            CE2 TYR
                                                 158 -342 1 9 7
ATOM
       896
            CZ TYR
ANISOU 896
            CZ
                 TYR
                                                 -146 -106 2 4 6
ATOM
       897
            OH TYR
ANISOU 897
            OH TYR
                                          2279
                                                 -87 -60 5 3
ATOM
       898
                 THR. 128 8.467
                                28.412 42.616 1.000 14.69
            N
ANISOU 898
            N
                 THR
                     128 1813
                                  1324 2446 -154 -217 2
28.984 42.011 1.000 14.67
                                                 -154 -217 2 6 8
                     128 1867
128 10
ATOM
       899
            CA THR
ANISOU 899
            CA THR
                                  1469
                                          2238
                     128 1867 1469 2238 -98 -32 1
128 10.921 28.552 42.736 1.000 14.68
                                                       -32 195
ATOM
       900
            C
                THR
ANISOU 900
                THR
                      128 1794
                                  1318
                                          2466
                                                 59 -123 -285
                      128 11.900 28.166 42.062 1.000 15.45
       901
            0
ATOM
                THR
ANISOU 901
            0
                THR
                      128 1715
                                  1487
                                          2667
                                                 -259 153 7 1
            CB THR
CB THR
OG1 THR
ATOM
       902
                                  30.544 42.069 1.000 16.02
                      128 9.572
ANISOU 902
                      128 2043
                                  1348
                                          2695
                                                 -79
                                                       59 4 7 9
                     128 8.519 30.849 41.162 1.000 19.14
ATOM
       903
ANISOU 903
            OG1 THR
                     128 2226
                                  2038
                                          3008
                                                 195
                                                      -23 545
            CG2 THR
ATOM
       904
                     128 10.835 31.187 41.582 1.000 19.03
ANISOU 904
                      128 2107
                                  1329
                                          3793
                                                 125
                                                       311 618
ATOM
       905
                      129 10.933 28.564 44.085 1.000 14.21
            N
                ALA
ANISOU 905
            N
                ALA
                      129 1708
                                         2424
                                  1266
                                                 -137
                                                       -256 - 181
ATOM
       906
            CA ALA
                     129 12.108 28.110 44.836 1.000 15.08
ANISOU 906 CA ALA
                      129 1670
                                  1435 2624 -118 -210 - 225
ATOM
       907
                     129 12.389 26.643 44.562 1.000 14.37
            С
                ALA
ANISOU 907 C
                ALA
                      129 1706
                                  1299
                                         2457 -159 -203 1 5 7
ATOM
       908 0
                     129 13.552 26.238 44.445 1.000 14.10
129 1758 1464 2137 -5 -244 -14
129 11.887 28.313 46.313 1.000 17.08
129 2132 1851 2506 -183 -514 -
                ALA
ANISOU 908 O
                ALA
                                  1464 2137 -5 -244 -148
       909 CB ALA
ATOM
ANISOU 909 CB ALA
                                  1851 2506 -183 -514 - 239
ATOM
       910 N
                      130 11.343
                SER
                                  25.819 44.553 1.000 14.18
ANISOU 910 N
                      130 1884
                SER
                                 1237 2267 -224 -257 1 7 3
24.375 44.351 1.000 15.44
ATOM
       911 CA SER
                      130 11.487
ANISOU 911 CA SER
                      130 1840
                                  1219
                                         2807 -115 -135 - 7
ATOM
       912 C
                      130 12.072
                SER
                                  24.114 42.965 1.000 14.45
ANISOU 912 C
                      130 1345
                SER
                                  1481
                                          2665 78 -796 -209
ATOM
       913 O SER
                     130 13.037
                                  23.329 42.807 1.000 14.43
ANISOU 913 O
                      130 1327
               SER
                                 1382 2773 -74 -246 1 7 2
23.677 44.663 1.000 17.54
       914 CB SER
ATOM
                     130 10.120
ANISOU 914
            CB SER
                     130 1555
130 9.268
                                  1225 3884 -379 -647 1 2 6
23.888 43.558 1.000 27.32
ATOM
       915
            OG SER
ANISOU 915
            OG SER
                      130 2321
                                  3168 4893 11 -1207 8 6 5
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					- 43 -		
ATOM	916	M	ARG	131 11.555	24.772	41.909	1.000 14.47
ANISOU	916	N	ARG	131 1421	1448	2628	161 -384 - 166
ATOM	917	CA	ARG	131 12.163	24.598		1.000 14.91
ANISOU	917	CA	ARG	131 1689	1452	2525	-4 -526 -341
MOTA	918	С	ARG	131 13.605	25.079		1.000 14.05
ANISOU	918	С	ARG	131 1772	1435	2132	-72 -381 - 173
ATOM	919	0	ARG	131 14.448	24.438		1.000 15.14
ANISOU	919	0	ARG	131 1829	1658	2267	-109 -170 - 230
ATOM	920	CB	ARG	131 11.349	25.316		1.000 15.77
ANISOU	920	CВ	ARG	131 1720	1613	2660	-54 -493 - 94
ATOM	921	CG	ARG	131 9.970	24.737		1.000 16.08
ANISOU	921	CG	ARG	131 1703	1695	2711	-13 -647 - 141
ATOM	922	CD	ARG	131 9.326	25.390		1.000 26.56
ANISOU	922	CD	ARG	131 3589	2689	3813	-1037 -2156 7 4 5
MOTA	923	ΝE	ARG	131 9.327	26.831		1.000 25.91
ANISOU		ΝE	ARG	131 2856	2814	4174	-979 -1682 1413
ATOM	924	CZ	ARG	131 8.472	27.716		1.000 31.86
ANISOU		CZ	ARG	131 3546	2861	5697	-254 -1094 2201
ATOM	925		ARG	131 7.467	27.244		1.000 31.34
ANISOU			ARG	131 5127	3636	3144	-1474 -458 -115
MOTA	926		ARG	131 8.633	29.032	38.235	1.000 40.12
ANISOU		NH2	ARG	131 3500	2831	8912	-582 -1620 1802
ATOM	927	И	ALA	132 13.893	26.186		1.000 13.42
ANISOU		N	ALA	132 1683	1385	2033	-85 -652 - 24
ATOM	928	CA	ALA	132 15.246	26.751		1.000 13.38
ANISOU		CA	ALA	132 1617	1443	2022	-16 -499 - 79
ATOM	929	С	ALA	132 16.225	25.808	41.837	1.000 13.37
ANISOU	929	C	ALA	132 1398	1365	2316	-93 -253 1 5 4
ATOM	930	0	ALA	132 17.306	25.586	41.328	1.000 14.43
ANISOU	930	Ö	ALA	132 1459	1772	2251	-91 -240 1 0 6
ATOM	931	CB	ALA	132 15.275	28.084		1.000 16.52
ANISOU	931	СВ	ALA	132 2019	1243	3014	-199 -366 - 236
ATOM	932	N	VAL	133 15.893	25.248		1.000 13.62
ANISOU		N	VAL	133 1522	1515	2139	-63 -362 8 6
ATOM	933	CA	VAL	133 16.839	24.363	43.689	
ANISOU ATOM	933	CA	VAL	133 1902	1566.	2179	120 -491 - 27
ANISOU	934	C	VAL	133 16.923	23.073	42.890	
ATOM	934 935	C	VAL	133 1390	1633	2690	-9 -220 -218
ANISOU		0	VAL	133 18.036	22.538	42.773	1.000 15.49
ATOM	936	СB	VAL VAL	133 1442 133 16.545	1814	2630	63 -193 - 9 9
ANISOU		CB	VAL		24.170		1.000 14.61
ATOM	937		VAL	133 1528 133 15.362	1789 23.267	2234	-45 -391 2 1 0
ANISOU			VAL	133 15.362			1.000 16.78
ATOM	938		VAL	133 17.766	2123 23.650	2708	-249 -437 - 81
ANISOU			VAL	133 17.766	1942		1.000 16.51
ATOM	939	N	ALA	134 15.840	22.583	2561	-61 -831 6 4
ANISOU		N	ALA	134 1605	1451	2160	1.000 13.73
ATOM	940	CA	ALA	134 15.951	21.369		-75 -397 1 8 5 1.000 14.21
ANISOU	940	CA	ALA	134 1505	1796	2100	116 -570 - 3 3
ATOM	941	C	ALA	134 16.838	21.618		1.000 15.07
ANISOU	941	C	ALA	134 1766	1511	2450	43 -292 1 7
ATOM	942	Ö	ALA	134 17.600	20.750		1.000 14.36
ANISOU	942	0	ALA	134 1555	1567	2333	-60 -286 5 2
ATOM	943	СВ	ALA	134 14.535	20.925		1.000 16.97
ANISOU	943	СВ	ALA	134 1472	1943	3031	12 -470 - 299
MOTA	944	N	ARG	135 16.752	22.808		1.000 15.48
ANISOU	944	N	ARG	135 1848	1600	2433	14 -341 - 2
ATOM	945	CA.	ARG	135 17.618	23.153		1.000 16.07
ANISOU		CA	ARG	135 2139	1230	2735	-138 -189 3 5
ATOM	946	C	ARG	135 19.082	23.057		1.000 15.70
					23.05/	50.555	1.000 13.70

- 44 -ANISOU 946 С ARG 135 2059 1370 2535 -134 27 121 MOTA 947 0 ARG 135 19.928 22.604 38.176 1.000 18.07 ANISOU 947 0 ARG 135 2317 2014 2534 108 256 276 MOTA 948 CE ARG 135 17.277 24.586 38.096 1.000 21.96 ANISOU 948 CB ARG 135 3936 1640 2767 -4 -1480 614 ATOM 949 CG 135 17.571 ARG 24.989 36.689 1.000 27.53 ANISOU 949 CG 135 5112 ARG 2482 2866 816 -610 5 9 5 ATOM 950 CDARG 135 16.930 26.332 36.393 1.000 23.27 ANISOU 950 CDARG 135 3548 2428 2865 148 61 1371 ATOM 951 NΞ ARG 135 15.551 26.309 35.928 1.000 22.68 ANISOU 951 NΕ ARG 135 3488 1575 3556 -116 167 297 MOTA 952 CZARG 135 14.520 26.858 36.562 1.000 25.90 ANISOU 952 ARG CZ135 3801 2165 3874 921 -506 -179 MOTA 953 NH1 ARG 135 14.708 27.515 37.702 1.000 23.50 ANISOU 953 NH1 ARG 135 3582 2378 2969 94 137 5 3 2 954 ATOM NH2 ARG 135 13.287 26.758 36.035 1.000 24.30 ANISOU 954 NH2 ARG 135 3520 2441 3272 -101 72 5 8 2 ATOM 955 Ν GLU 136 19.403 23.533 40.149 1.000 15.76 ANISOU 955 Ν GLU 136 1897 1696 2396 -178 17 3 1 8 MOTA 956 CAGLU 136 20.752 23.431 40.694 1.000 15.16 ANISOU 956 CAGLU 136 1687 1770 2302 -97 279 140 ATOM 957 С 136 21.186 22.001 GLU 40.978 1.000 16.74 ANISOU 957 С GLU 136 1535 1704 3122 -148 -172 -72ATOM 958 0 GLU 136 22.350 21.637 40.701 1.000 17.42 ANISOU 958 0 GLU 136 1710 1908 2999 7 30 9 2 ATOM 959 CB GLU 136 20.957 24.284 41.962 1.000 16.64 ANISOU 959 CB GLU 136 2048 1785 2487 53 11 - 16 960 ATOM CG GLU 136 20.762 25.772 41.718 1.000 17.80 ANISOU 960 CG GLU 136 2036 1714 3014 -286 -169 1 1 0 961 ATOM CDGLU 136 21.534 26.269 40.513 1.000 20.92 ANISOU 961 CD GLU 136 2174 2273 3503 -343 70 4 6 9 ATOM 962 OE1 GLU 136 22.742 25.987 40.454 1.000 24.97 ANISOU 962 OE1 GLU 136 2116 2434 4938 -494 531 219 963 MOTA OE2 GLU 136 21.022 27.037 39.672 1.000 24.77 ANISOU 963 OE2 GLU 136 2975 2618 3817 -708 -133 1029 MOTA 964 Ν VAL 137 20.262 21.172 41.450 1.000 15.34 ANISOU 964 N VAL 137 1681 1696 2453 -108 -287113ATOM 965 CAVAL 137 20.568 19.750 41.647 1.000 15.92 ANISOU 965 CA137 1755 VAL 1802 2493 83 -4 2 1 0 MOTA 966 C VAL 137 20.926 19.086 40.326 1.000 15.86 ANISOU 966 C VAL 137 1604 1869 2555 -38 -35 6 6 MOTA 967 137 21.905 18.308 0 VAL 40.174 1.000 16.70 ANISOU 967 0 137 1617 VAL 2118 72 -151 - 90 2609 ATOM 968 CB VAL 137 19.358 18.990 42.283 1.000 15.35 ANISOU 968 CB VAL 137 1729 1663 2440 8 -29 5 ATOM 969 CG1 VAL 137 19.607 17.478 42.176 1.000 16.93 ANISOU 969 137 1521 CG1 VAL 1689 3223 -345 9 6 160 MOTA 970 CG2 VAL 137 19.144 19.420 43.724 1.000 15.43 ANISOU 970 CG2 VAL 137 1529 2090 2245 -277 1 8 5 ~53 ATOM 971 N 138 20.149 19.407 LEU 39.284 1.000 15.52 ANISOU 971 Ν LEU 138 1625 1735 2535 -105 -61 109 972 CALEU 138 20.378 18.881 37.936 1.000 15.74 ANISOU 972 ÇA LEU 138 1576 1862 2543 -71 15 5 1 ATOM 973 C 138 21.721 19.396 LEU 37.406 1.000 17.42 ANISOU 973 С LEU 138 1588 2119 2912 -87 162 ATOM 974 0 LEU 138 22.503 18.609 36.846 1.000 19.13 ANISOU 974 0 LEU 138 1878 2406 2985 186 317 MOTA 975 CB LEU 138 19.211 19.248 36.996 1.000 14.70 ANISOU 975 CB LEU 138 1592 1642 2349 -50 141 MOTA 976 CG LEU 138 17.883 18.541 37.375 1.000 14.38 ANISOU 976 CG LEU 138 1657 1409 2399 -44

- 45 -MOTA 977 CD1 LEU 138 16.774 19.122 36.491 1.000 16.13 ANISOU 977 CD1 LEU 138 1743 2539 1848 -218 1 6 8 128 978 CD2 LEU 138 17.975 17.027 37.156 1.000 17.48 ANISOU 978 138 2185 CD2 LEU 1435 3021 -107 -480 287 979 139 21.963 MOTA N ARG 20.708 37.548 1.000 17.44 ANISOU 979 N ARG 139 1797 2157 2674 -319 238 192 980 ATOM CA ARG 139 23.189 21.319 36.996 1.000 19.06 ANISOU 980 CA ARG -366 139 2043 2462 2735 482 376 981 C MOTA ARG 37.685 1.000 19.72 139 24.419 20.734 ANISOU 981 С ARG 139 1797 2600 3097 -518 482 376 ATOM 982 0 ARG 139 25.461 20.432 37.094 1.000 20.70 ANISOU 982 0 ARG 139 2046 2469 3350 -288 607 195 ATOM 983 CB ARG 139 23.152 22.850 37.101 1.000 24.54 ANISOU 983 CB ARG 139 2525 2403 4396 -402 951 690 984 139 23.886 23.665 36.073 1.000 36.05 ATOM CG ARG ANISOU 984 CG ARG 139 6517 2967 4212 -2176 1609 1 4 0 985 CD ARG 139 23.852 25.148 36.443 1.000 44.95 ATOM CD ARG NE ARG ANISOU 985 139 7459 1902 7716 -242 -1324 1930 ATOM 986 139 22.525 25.727 36.547 1.000 43.27 ANISOU 986 NE ARG 139 6637 3846 5959 -828 -2173 -698 ARG CZATOM 987 139 21.821 26.330 35.605 1.000 41.34 ARG ANISOU 987 CZ139 5939 4102 5666 497 645 1 139 22.308 26.436 34.376 1.000 44.01 645 1140 NH1 ARG ATOM 988 ANISOU 988 139 6564 4146 6011 550 1393 3 139 20.614 26.837 35.833 1.000 45.75 NH1 ARG 1393 3 3 6 ATOM 989 NH2 ARG ANISOU 989 NH2 ARG 139 6162 4618 6602 537 1938 2 140 24.357 20.566 39.009 1.000 18.77 1938 2405 ATOM 990 ALA N ANISOU 990 ALA N 140 :1742 3003 -255 145 6 9 2387 20.169 39.773 1.000 19.53 MOTA 991 CA ALA 140 25.532 CA ALA ANISOU 991 140 1583 2641 3197 -28 38 - 668 ATOM 992 C 140 25.932 18.732 ALA 39.490 1.000 18.96 ANISOU 992 C 140 2018 ALA 2342 2843 -67 76 - 103 ATOM 993 0 140 27.109 18.335 39.626 1.000 21.36 ALA ANISOU 993 0 ALA 140 1900 2436 3778 -2 472 - 80 ATOM 994 CB ALA 140 25.273 20.345 41.275 1.000 19.74 ANISOU 994 CB ALA 140 1824 2592 3084 35 0 - 360 995 N MOTA THR 141 24.958 17.943 39.062 1.000 20.32 ANISOU 995 N THR 141 2014 2209 3498 -115 305 -138 ATOM 996 CA THR 141 25.151 16.530 38.717 1.000 17.15 ANISOU 996 CA THR ATOM 997 C THR 141 1870 2039 2609 61 51 2 1 8 141 25.269 16.278 37.208 1.000 17.44 ANISOU 997 С THR 141 1492 2443 2693 21 278 1 9 9 ATOM 998 0 THR 141 25.343 15.106 36.792 1.000 19.24 ANISOU 998 0 THR 141 1871 2623 2814 63 579 - 63 CB THR MOTA 999 141 24.048 15.629 39.290 1.000 16.79 ANISOU 999 141 1708 2261 2410 83 164 3 1 ATOM 1000 OG1 THR 141 22.788 16.012 38.710 1.000 17.18 ANISOU 1000 OG1 THR 141 1894 2235 2399 -101 -53 518 ATOM 1001 CG2 THR 141 23.982 15.734 40.807 1.000 17.83 ANISOU 1001 CG2 THR 141 1521 2878 2377 -43 2 0 164 MOTA 1002 N GLY 142 25.361 17.301 36.381 1.000 19.69 ANISOU 1002 N GLY 142 2091 2789 2603 -708 302 297 ATOM 1003 CA GLY 142 25.517 17.123 34.923 1.000 19.08 ANISOU 1003 CA GLY142 1878 2819 2551 128 -163 2 5 5 ATOM 1004 C GLY 142 24.284 16.441 34.313 1.000 18.75 ANISOU 1004 C GLY 142 1972 2410 2744 0 252 - 117 1005 O ATOM GLY 142 24.443 15.755 33.315 1.000 22.41 ANISOU 1005 O GLY 142 2432 2681 3403 -161 571 -680 1006 N ATOM THR 143 23.093 16.650 34.854 1.000 17.28 ANISOU 1006 N THR 143 1895 2002 2667 67 300 2 4 4 1007 CA THR ATOM 143 21.909 15.932 34.393 1.000 16.88

- 46 -ANISOU 1007 CA THR 143 1953 2006 2456 164 332 THR 143 20.998 16.660 33.432 1.000 17.02 1008 C ANISOU 1008 C THR 143 2149 1795 2521 82 196 1 1 7 1009 0 THR 143 20.457 17.713 33.764 1.000 20.30 ATOM 143 2795 1815 3103 344 12 - 2 8 143 21.085 15.490 35.623 1.000 16.40 ANISOU 1009 O THR 12 - 28 MOTA 1010 CB THR ANISOU 1010 CB THR 143 1755 2329 2148 -37 95 - 44 1011 OG1 THR 143 21.922 14.692 36.479 1.000 17.82 MOTA
 143
 2009
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 -109
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 33
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 143
 19.887
 14.621
 35.270
 1.000
 19.51

 143
 1957
 2290
 3167
 -192
 -94
 100

 144
 20.742
 16.070
 32.248
 1.000
 18.79

 144
 2138
 2203
 2800
 47
 12
 -121
 ANISOU 1011 OG1 THR 1012 CG2 THR MOTA ANISOU 1012 CG2 THR 1013 N GLU ANISOU 1013 N GLU 144 19.729 16.573 1014 CA 31.334 1.000 20:13 GLU MOTA 144 2202 ANISOU 1014 CA GLU 2696 2750 -292 -41 316 144 18.637 15.506 31.254 1.000 19.18 1015 C MOTA GLU GLU ANISOU 1015 C -292 144 2255 2614 2418 230 -131 144 18.827 14.438 30.665 1.000 21.46 ATOM 1016 0 GLU ANISOU 1016 O 144 2268 GLU 2442 3446 19 649 - 88 1017 CB AGLU 144 20.250 17.061 30.006 0.753 29.50 ANISOU 1017 CB AGLU 144 3376 4266 3566 -855 206 1501 AGLU 144 20:195 18.567 29.741 0.753 36.54 1018 CG ANISOU 1018 CG AGLU 144 6059 3913 3913 -1728 1769 7 9 5 ATOM 1019 CD AGLU 144 21.242 19.411 30.426 0.753 33.13 ANISOU 1019 CD AGLU 144 4189 3432 4966 104 744 884 1020 OE1AGLU 144 21.079 19.690 31.641 0.753 51.91 ATOM ANISOU 1020 OE1AGLU 144 3684 11101 4940 -868 -202 - 590 1021 OE2AGLU 144-22.207 19.910 29.807 0.753 50.79 1021 OE2AGLU 144 7949 3695 7653 -3071 3099 - 1022 CB BGLU 144 20.372 16.724 29.951 0.247 18.36 ANISOU 1021 OE2AGLU 7653 -3071 3099 -1249 BGLU 144 868 3091 3016 334 16 2 6 2 BGLU 144 21.214 17.988 29.779 0.247 23.54 BGLU 144 1301 3586 4056 -38 595 5 BGLU 144 21.150 18.468 28.336 0.247 33.24 ANISOU 1022 CB ATOM 1023 CG ANISOU 1023 CG 1024 CD MOTA ANISOU 1024 CD BGLU 144 3589 3975 438 5064 -20 144 20.417 17.818 ATOM 1025 OE1BGLU 27.557 0.247 28.68 144 3222 ANISOU 1025 OE1BGLU 2861 1729 1280 4813 389 1026 OE2BGLU 144 21.814 19.464 27.990 0.247 35.35 ATOM ANISOU 1026 OE2BGLU 144 3176 5108 35 1752 5148 1516 1027 N 145 17.508 15.724 31.911 1.000 17.11 MOTA PRO ANISOU 1027 N PRO 145 2132 1825 2543 68 62 1 5 8 1028 CA PRO 145 16.396 14.781 31.846 1.000 17.41 ANISOU 1028 CA PRO 145 2290 1942 2384 -73 400 1 2 145 15.966 14.545 30.406 1.000 17.94 ATOM 1029 C PRO ANISOU 1029 C PRO 145 2386 1955 2475 -116 292 -1041030 0 MOTA PRO 145 16.068 15.439 29.557 1.000 18.26 ANISOU 1030 O PRO 145 2271 -272 170 4 5 2196 2472 1031 CB PRO 145 15.250 15.493 32.594 1.000 17.07 ATOM ANISOU 1031 CB PRO 145 2181 2534 35 133 - 143 1771 1032 CG PRO MOTA 145 15.950 16.504 33.464 1.000 17.11 ANISOU 1032 CG PRO 145 2341 2319 23 -49 - 24 1841 ATOM 1033 CD PRO 145 17.131 16.977 32.649 1.000 17.54 ANISOU 1033 CD 145 2178 PRO 1601 2884 178 -88 3 0 3 1034 N MOTA ASP 146 15.490 13.346 30.104 1.000 18.15 ANISOU 1034 N ASP 146 2140 321 -152 1965 2790 -60 ATOM 1035 CA ASP 146 14.909 13.121 28.775 1.000 18.43 ANISOU 1035 CA ASP 146 2487 1664 2853 -329 310 -156 ASP MOTA 1036 C 146 13.809 14.154 28.566 1.000 18.07 146 12.959 14.333 29.422 1.000 18.29 146 2491 2173 2287 -169 202 ANISOU 1036 C ASP 208 - 3091037 0 MOTA ASP ANISOU 1037 O ASP 203 - 230

- 47 -1038 CB ASP 146 14.221 11.735 28.717 1.000 23.50 ATOM ANISOU 1038 CB ASP 146 3489 1038 CB ASP 146 3489 1671 3769 -653 908 -665 1039 CG ASP 146 13.636 11.508 27.334 1.000 34.15 ATOM 1040 OD1 ASP 146 4070 4205 4700 -1004 361 -2386 ANISOU 1040 OD1 ASP 146 3971 9175 3849 2177 677 ATOM ATOM 1041 OD2 ASP 146 3971 9175 3849 -2156 683 3 7 8 ANISOU 1041 OD2 ASP 146 14.421 11.229 26.397 1.000 44.78 ATOM 1042 N GLY 147 13 001 GLY 147 2622 2331 2374 527 78 140 4342 8626 4046 -813 289 -2326 GLY 147 2622 2331 2374 527 78 ANISOU 1042 N ATOM 1042 N GLY 147 2622 2331 2374 -635. -72 1 1 3 ANISOU 1043 CA GLY 147 12.916 15.878 27.171 1.000 18.58 ANISOU 1044 C GLY 147 13.335 17.262 27.590 1.000 18.25 ANISOU 1044 C GLY 147 2511 2432 1993 -335 -138 6 4 ATOM 1045 O GLY 147 2511 2432 1993 -335 -138 6 4 ATOM 1045 O GLY 147 2469 2739 2673 -282 -144 2 0 5 ATOM 1046 N GLY 147 2469 2739 2673 -282 -144 2 0 5 ATOM 1046 N GLY 148 18.027 18.658 28.6672 1.000 17.38 ANISOU 1047 CA GLY 148 185.027 18.658 28.6672 1.000 16.72 ANISOU 1047 CA GLY 148 185.027 18.658 28.672 1.000 13.94 ATOM 1047 CA GLY 148 185.027 18.658 28.672 1.000 13.94 ATOM 1049 O GLY 148 185.77 1645 2135 77 -201 117 ATOM 1049 O GLY 148 18.157 1645 2135 77 -201 117 ATOM 1050 N VAL 149 15.431 20.003 30.641 1.000 16.29 ANISOU 1049 O GLY 148 1839 1863 2487 -151 -77 28 5 ATOM 1051 CA VAL 149 15.275 20.509 30.641 1.000 14.93 ANISOU 1051 CA VAL 149 15.275 20.509 30.641 1.000 14.37 ATOM 1052 C VAL 149 13.958 21.218 32.225 1.000 14.37 ATOM 1053 O VAL 149 15.431 20.003 30.641 1.000 14.36 ATOM 1053 O VAL 149 15.439 21.218 32.225 1.000 14.37 ATOM 1054 CB VAL 149 13.203 20.970 33.163 1.000 14.37 ATOM 1055 CG1 VAL 149 13.203 20.970 33.163 1.000 14.37 ATOM 1055 CG1 VAL 149 16.349 21.218 32.225 1.000 14.37 ATOM 1055 CG1 VAL 149 16.228 22.101 33.752 1.000 14.37 ATOM 1055 CG1 VAL 149 16.228 22.101 33.752 1.000 14.37 ATOM 1055 CG1 VAL 149 16.228 22.101 33.752 1.000 15.26 ATOM 1055 CG2 VAL 149 17.35 1044 2682 -39 83 1.88 ATOM 1055 CG1 VAL 149 16.228 22.101 33.752 1.000 16.66 ATOM 1055 CG1 VAL 149 16.228 22.101 33.752 1.000 17.65 ATOM 1055 CG1 VAL 149 16.228 22.101 33.752 1.000 15.26 ATOM 1055 CG1 VAL 149 16.228 22.101 33.752 1.000 15.26 ATOM 1055 CG1 VAL 149 15.03 15.01 1043 CA GLY 147 12.916 15.878 27.171 1.000 18.58 ANISOU 1043 CA GLY 147 2463 1062 CG GLU 150 13.761 25.167 31.220 1.000 19.00 ATOM 1062 CG GLU 150 13.761 25.167 31.220 1.000 19.00 ANISOU 1062 CG GLU 150 2483 1212 3523 -65 -95 4 6 5 ATOM 1063 CD GLU 150 13.810 25.624 32.658 1.000 20.32 ANISOU 1063 CD GLU 150 2444 1746 3532 -130 -24 4 5 4 ATOM 1064 OE1 GLU 150 12.781 25.749 33.377 1.000 20.88 ANISOU 1064 OE1 GLU 150 2558 1728 3648 29 58 3 9 6 ATOM 1065 OE2 GLU 150 14.913 25.946 33.161 1.000 21.77 ANISOU 1065 OE2 GLU 150 2549 2030 3693 -165 -202 2 7 3 ATOM 1066 N ALA 151 11.050 21.288 30.603 1.000 14.98 ANISOU 1066 N ALA 151 1649 1710 2334 37 -307 5 5 1 ATOM 1067 CA ALA 151 9.834 20.475 30.543 1.000 15.79 ANISOU 1067 CA ALA 151 1820 2045 2136 -173 -198 4 0 8 ATOM 1068 C ALA 151 9.748 19.531 31.724 1.000 15.38

- 48 -

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ANISOU 1069 O ALA 151 1778
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ATOM
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ANISOU 1091 CA ASP
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- 50 -ANISOU 1129 CA LEU 159 1438 1555 2095 -36 -80 - 91 1130 C LEU 159 0.419 21.494 49.602 1.000 14.49 1130 C LEU 159 1336 2034 2135 -152 -20S -MOTA ANISOU 1130 C 159 1336 2034 2135 -152 -20S - 38 159 -0.790 21.596 49.419 1.000 15.09 ATOM 1131 0 LEU ANISOU 1131 O LEU 159 1414 1999 2319 90 -131 9 0 ATOM 1132 CB LEU 159 1.390 23.466 48.394 1.000 15.28 ANISOU 1132 CB LEU 159 1720 1447 2639 55 -325 -197 1133 CG 159 1.484 24.320 49.669 1.000 17.11 LEU ANISOU 1133 CG LEU 159 2146 1689 2665 363 -332 -159 2.775 24.114 50.453 1.000 18.70 -332 - 343 MOTA 1134 CD1 LEU ANISOU 1134 CD1 LEU 159 2276 1759 3070 379 -687 - ATOM 1135 CD2 LEU 159 1.312 25.801 49.291 1.000 21.00 ATOM 1136 N ARG 160 0.916 21.107 50.774 1.000 14.37 -687 - 540 -692 - 382 ATOM 1136 N ARG 160 0.916 21.107 50.774 1.000 14.37 ANISOU 1136 N ARG 160 1688 1709 2063 -101 -186 4 7 ANISOU 1137 CA ARG 160 0.055 20.747 51.901 1.000 15.61 ATOM 1138 C ARG 160 0.480 21.501 53.155 1.000 15.40 ANISOU 1138 C ARG 160 1557 2158 2135 -34 -46 -38 ANISOU 1139 O ARG 160 1.639 21.401 53.576 1.000 16.32 ATOM 1140 CB ARG 160 0.048 19.263 52.227 1.000 16.13 ANISOU 1140 CB ARG 160 2134 2084 1912 -127 -30 129 ATOM 1141 CG ARG 160 -0.594 18.410 51.155 1.000 17.17 ARG 160 -0.594 18.410 51.155 1.000 17.17 ARG 160 1963 1934 2628 -140 -212 -ANISOU 1141 CG 2628 -140 -212 - 60 160 -0.672 16.959 51.627 1.000 18.16 ATOM 1142 CD ARG ANISOU 1142 CD ARG 160 2767 1965 2166 125 -330 - 35 160 2767 1963 2160 123 -333 1602 -1.382 16.102 50.682 1.000 18.11 1143 NE ARG ANISOU 1143 NE ARG 160 2408 1775 2699 **-**56 -308 2 0 ATOM 1144 CZ 160 -1.221 14.789 50.581 1.000 16.76 ARG 1144 CZ ARG 160 2191 1748 2428 -97 55 174
1145 NH1 ARG 160 -0.326 14.192 51.374 1.000 20.55 ANISOU 1144 CZ ARG ANISOU 1145 NH1 ARG 160 2306 2012 3491 -26 -457 3 0 5 ATOM 1146 NH2 ARG 160 -1.908 14.095 49.689 1.000 19.23 ANISOU 1146 NH2 ARG 160 2502 2031 2774 181 -147 - 3 3 AKG 160 2502 2031 2774 181 -147 - PHE 161 1604 2120 2111 37 -147 - 3381147 N ANISOU 1147 N 1147 N PHE 161 1604 2120 2111 -37 -63 -1148 CA PHE 161 -0.209 22.975 54.999 1.000 16.25 -63 -128 ATOM ANISOU 1148 CA PHE 161 2173 1774 2227 -71 -187 - 891149 C PHE 161 -1.030 22.236 56.069 1.000 16.98 ATOM ANISOU 1149 C PHE 161 1980 2432 2041 -217 -161 -162 ATOM PHE 161 -2.248 22.113 55.948 1.000 20.38 PHE 161 1981 3291 2473 -190 -191 - 72 1150 O ANISOU 1150 O 1151 CB PHE 161 -0.683 24.431 54.862 1.000 19.76 161 2065 1903 3540 167 355 -ANISOU 1151 CB PHE 161 2065 1903 3540 167 355 -198 161 -0.379 25.259 56.109 1.000 23.61 161 3026 1905 4041 836 -59 -591 161 -1.194 25.304 57.228 1.000 28.25 161 3992 2474 4268 1077 369 -1253 161 0.807 25.978 56.141 1.000 26.62 161 4015 2483 3616 -130 -927 -106 161 -0.850 25.992 58.383 1.000 35.29 3540 167 355 -198 1152 CG PHE ATOM ANISOU 1152 CG PHE 1153 CD1 PHE ATOM ANISOU 1153 CD1 PHE 1077 369 -1253 ATOM 1154 CD2 PHE ANISOU 1154 CD2 PHE ATOM 1155 CE1 PHE 1155 CE1 PHE 161 -0.850 25.992 58.383 1.000 35.29 1155 CE1 PHE 161 6873 2097 4437 1538 -135 -1399 1156 CE2 PHE 161 1.153 26.723 57.258 1.000 33.63 1157 CZ PHE 161 0.320 26.726 53.363 1.000 36.44 1158 N ARG 162 -0.358 21.767 57.130 1.000 17.59 1159 CA ARG 162 2769 2414 1758 6 178 - 378 ANISOU 1155 CE1 PHE ATOM ANISOU 1156 CE2 PHE ANISOU 1157 CZ PHE MOTA ANISOU 1158 N ATOM ANISOU 1159 CA ARG

- 51 -1160 C MOTA ARG 162 -0.880 21.758 59.553 1.000 20.16 162 2110 3341 2210 -36 41 -96 162 0.217 22.160 59.893 1.000 19.61 162 2257 2993 2201 -194 -73 -1 ANISOU 1160 C ARG ATOM 1161 0 ARG ANISOU 1161 O ARG 2201 -194 - 73 - 359162 -0.580 19.640 58.356 1.000 20.81 ATOM 1162 CB ARG ANISOU 1162 CB ARG 162 2958 2275 2675 -129 6 -169 162 -0.843 18.724 57.166 1.000 19.90 1163 CG ARG ATOM ANISOU 1163 CG ARG 162 3044 2073 2443 -112 254 - 38 162 3044 20/3 2443 -112 254 -162 -0.182 17.383 57.393 1.000 28.02 1164 CD ARG ANISOU 1164 CD ARG 162 5599 2038 3010 381 -14 114 1165 NE ARG 162 -0.369 16.420 56.326 1.000 27.74 ANISOU 1165 NE ARG 1165 NE ARG 162 4151 2294 15.445 1166 CZ ARG 162 -1.278 15.445 16.370 1.000 31.11 1166 CZ ARG 162 2560 3729 5531 470 -350 -162 4151 -687 -434 ATOM ANISOU 1166 CZ ARG 162 2560 -350 -1152 1167 NH1 ARG 162 -2.092 15.324 57.403 1.000 42.97 1167 NH1 ARG 162 3475 5906 6946 -579 1019 -ATOM ANISOU 1167 NH1 ARG 162 3475 5906 6946 -579 1019 -2492 1168 NH2 ARG 162 -1.329 14.603 55.353 1.000 29.64 1168 NH2 ARG 162 3066 2738 5458 120 -143 -ATOM ANISOU 1168 NH2 ARG 162 3066 -143 - 7081169 N TYR 163 -1.956 21.780 60.311 1.000 19.52 1169 N TYR 163 2394 2901 2120 147 263 -MOTA ANISOU 1169 N ATOM 1170 CA TYR 163 -1.943 22.102 61.732 1.000 22.74 ANISOU 1170 CA TYR 163 3312 3107 2219 369 302 -ANISOU 1170 CA TYR 163 3312 3107 2219 369 302 -878 ATOM 1171 C TYR 163 -2.037 20.800 62.536 1.000 24.20 ANISOU 1171 C TYR 163 2802 3901 2492 -222 253 -189 ATOM 1172 O TYR 163 -2.992 20.049 62.274 1.000 28.02 ANISOU 1172 O TYR 163 2305 4409 3934 -202 -126 3 9 9 ATOM 1173 CB TYR 163 -3.198 22.912 62.114 1.000 28.98 ANISOU 1173 CB TYR 163 -3.342 22.912 62.114 1.000 28.98 ANISOU 1174 CG TYR 163 -3.342 22.997 63.623 1.000 25.58 ANISOU 1174 CG TYR 163 2572 3382 3767 543 749 -1204 ATOM 1175 CD1 TYR 163 -2.458 23.826 64.319 1.000 37.32 ANISOU 1175 CD1 TYR 163 3654 6112 4413 -759 884 -23.73 302 - 878 ANISOU 1175 CD1 TYR 163 3654 6112 4413 -759 884 -2373 163 -4.315 22.333 64.345 1.000 29.13 ATOM 1176 CD2 TYR ANISOU 1176 CD2 TYR 163 2622 3994 4452 749 1084 - 769 163 -2.546 23.966 65.702 1.000 38.28 1177 CE1 TYR ANISOU 1177 CE1 TYR 163 2905 7138 4503 -454 987 -2740 163 -4.396 22.431 65.726 1.000 37.36 1178 CE2 TYR 1178 CE2 TYR 163 3220 6336 4640 -273 1997 -1618 1179 CZ TYR 163 -3.500 23.250 66.393 1.000 49.85 1179 CZ TYR 163 5272 8795 4872 -1810 1593 -2223 1180 OH TYR 163 -3.595 23.365 67.768 1.000 44.81 ANISOU 1178 CE2 TYR ATOM ANISOU 1179 CZ ATOM ANISOU 1180 OH TYR 163 5246 7368 4413 -222 270 -496 ATOM 1181 N PHE 164 -1.098 20.651 63.448 1.000 24.84 ANISOU 1181 N PHE 164 2905 3368 3164 -89 -125 - 361 ATOM 1182 CA PHE 164 -1.045 19.532 64.370 1.000 28.14 ANISOU 1182 CA PHE 164 3538 3957 3195 223 -163 - 30 164 -1.360 20.003 65.787 1.000 26.67 164 2964 3937 3234 -473 -194 - 257 ATOM 1183 C PHE ANISOU 1183 C PHE 164 -0.540 20.730 66.342 1.000 31.26 ATOM 1184 0 PHE ANISOU 1184 O PHE 164 3119 4888 3869 -959 -260 -5

ATOM 1185 CB PHE 164 0.347 18.881 64.396 1.000 27.86

ANISOU 1185 CB PHE 164 3423 3725 3436 76 -199 - 32

ATOM 1186 CG PHE 164 0.744 18.301 63.052 1.000 26.77

ANISOU 1186 CG PHE 164 2914 3474 3785 -598 74 -27

ATOM 1187 CD1 PHE 164 1.435 19.093 62.143 1.000 26.16 3869 -959 -260 -519 3436 76 -199 - 32 3785 -598 74 - 275 ANISOU 1187 CD1 PHE 164 2827 3836 3278 135 -615 7 1 1 1188 CD2 PHE MOTA 164 0.414 16.996 62.717 1.000 31.24 ANISOU 1188 CD2 PHE 164 4365 2808 4698 349 -298 - 96 ATOM 1189 CE1 PHE 164 1.787 18.609 60.894 1.000 30.09 ANISOU 1189 CE1 PHE 164 3609 5052 2771 -148 -1030 641 MOTA 1190 CE2 PHE 164 0.786 16.501 61.475 1.000 38.25

- 52 -ANISOU 1190 CE2 PHE 164 6659 4077 3797 -740 -1363 -612 1191 CZ PHE 164 1.494 17.298 60.588 1.000 32.74 PHE 164 3189 ANISOU 1191 CZ 5078 4172 712 -944 - 385 165 -2.469 19.609 1192 N PRO 66.379 1.000 30.62 ANISOU 1192 N PRO 165 3876 4009 3751 -1371 344 -508 1193 CA PRO MOTA 165 -2.670 19.813 67.809 1.000 33.09 ANISOU 1193 CA PRO 165 3299 5764 3510 -190 80 2 3 6 1194 C PRO 165 -1.459 19.408 68.638 1.000 36.32 ATOM ANISOU 1194 C PRO 165 3538 5745 4518 664 -191 - 234165 -0.776 18.428 1195 0 PRO MOTA 68.371 1.000 32.94 ANISOU 1195 O PRO 165 4268 4761 3487 220 501 387 1196 CB PRO 165 -3.882 18.929 ATOM 68.123 1.000 38.44 ANISOU 1196 CB PRO 165 3807 6924 3873 -765 271 827 ATOM 1197 CG PRO 165 -4.635 18.842 66.845 1.000 35.82 PRO 165 2595 ANISOU 1197 CG 7020 5 688 - 828 3995 1198 CD ATOM PRO 165 -3.690 19.130 65.710 1.000 33.90 ANISOU 1198 CD PRO 165 3192 5919 3770 -1149 194 1 6 9 1199 N LEU 178 7.727 7.453 68.180 1.000 64.52 178 7.727 7.453 178 12297 5376 178 7.629 8.260 178 10557 2730 178 6.159 8.539 178 9239 3530 178 5.314 7.659 178 11777 5626 178 8.222 7.582 178 11470 3734 ANISOU 1199 N LEU 6843 278 -218 3721 MOTA 1200 CA LEU 66.973 1.000 43.31 ANISOU 1200 CA LEU 3168 -984 -2821 -135 MOTA 1201 C LEU 66.662 1.000 47.36 ANISOU 1201 C LEU 5225 -2598 -1186 1204 MOTA 1202 0 LEU 66.796 1.000 56.53 ANISOU 1202 O LEU 4076 -4835 1265 -602 MOTA 1203 CB LEU 65.746 1.000 55.55 178 11470 3734 ANISOU 1203 CB LEU 5902 -1314 -1197 -1822 178²9.662 7.092 1204 CG LEU 65.774 1.000 62.34 178 10812 5116 ANISOU 1204 CG LEU 7760 -1971 194 - 443 178 9.916 6.185 ATOM 1205 CD1 LEU 64.579 1.000 54.23 ANISOU 1205 CD1 LEU 178 9626 4989 5988 1878 -3799 511 178 10.633 8.264 ATOM 1206 CD2 LEU 65.773 1.000 66.44 ANISOU 1206 CD2 LEU 178 11265 3454 10526 -1170 4090 -516 1207 N ATOM ARG 179 5.879 9.751 66.192 1.000 52.90 ANISOU 1207 N 179 7853 3826 ARG 8421 102 1230 1031 1208 CA ARG ATOM 179 4.495 10.033 65.807 1.000 51.26 ANISOU 1208 CA ARG 179 7235 4820 7421 -229 1890 - 383 ATOM 1209 C ARG 179 4.242 9.563 64.383 1.000 55.25 ANISOU 1209 C 179 7178 6083 ARG 7731 -946 2260 -1134 1210 0 ATOM . 179 3.120 9.211 ARG 64.021 1.000 58.51 ANISOU 1210 O 179 7036 ARG 7628 7565 -1820 3675 -2851 MOTA 1211 CB 179 4.180 11.512 66.040 1.000 41.49 ARG ANISOU 1211 CB ARG 179 6600 4448 4716 -155 1916 1137 179 3.293 11.700 ATOM 1212 CG ARG 67.277 1.000 43.15 179 6120 5908 179 1.888 12.059 ANISOU 1212 CG ARG 4367 90 1338 530 ATOM 1213 CD ARG 66.833 1.000 47.63 ANISOU 1213 CD ARG 179 6180 7453 4463 195 860 - 531 ATOM 1214 NE ARG 179 1.459 13.367 67.269 1.000 52.00 ANISOU 1214 NE 179 7384 ARG 7834 4539 1669 -1168 -538 ATOM 1215 CZ ARG 179 1.322 14.470 66.556 1.000 64.81 ANISOU 1215 CZ 179 10838 179 1.637 ARG 8000 5788 1457 -1107 6 3 1216 NH1 ARG ATOM 14.518 65.268 1.000 59.74 ANISOU 1216 NH1 ARG 179 9535 8090 5074 3628 -2691 ATOM 1217 NH2 ARG 179 0.907 15.606 67.117 1.000 65.83 ANISOU 1217 NH2 ARG 179 10451 9083 5478 4171 -776 1200 ATOM 1218 N . MET 180 5.304 9.501 63.589 1.000 43.96 ANISOU 1218 N MET 180 5383 3769 7550 705 852 - 1245 1219 CA MET 180 5.264 9.035 62.210 1.000 40.44 ANISOU 1219 CA MET 180 2356 5467 7543 -398 574 -1482 ATOM 1220 C MET 180 6.552 61.920 1.000 43.91 8.258 ANISOU 1220 C MET 180 2731 7733 6220 18 320 - 2324

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ATOM 1238 N HIS 183 10.111 7.414 56.561 1.000 19.27 ANISOU 1238 N HIS 183 2131 2658 2533 -274 -204 1 7 6 ATOM 1239 CA HIS 183 9.757 7.306 55.144 1.000 18.01 ANISOU 1239 CA HIS 183 1882 2311 2652 -341 -455 3 4 6 ATOM 1240 C HIS 183 10.749 8.124 54.337 1.000 15.74 ANISOU 1240 C HIS 183 1964 1560 2456 -75 -352 1 2 8 ATOM 1241 O HIS 183 11.355 9.061 54.868 1.000 18.14 ANISOU 1241 C HIS 183 2297 2093 2504 -509 -127 -135 ATOM 1242 CB HIS 183 8.338 7.781 54.835 1.000 18.66 ANISOU 1242 CB HIS 183 1970 2173 2945 -136 -243 3 7 1 ATOM 1243 CG HIS 183 8.089 9.120 55.447 1.000 26.67 ANISOU 1244 ND1 HIS 183 7.884 9.362 56.800 1.000 35.36 ANISOU 1244 ND1 HIS 183 7.884 9.362 56.800 1.000 35.36 ANISOU 1245 CD2 HIS 183 8.051 10.311 54.821 1.000 33.00 ANISOU 1245 CD2 HIS 183 4432 4078 4926 -1190 1466 -1454 ATOM 1245 CD2 HIS 183 7.739 10.658 56.980 1.000 35.91 ANISOU 1246 CE1 HIS 183 7.739 10.658 56.980 1.000 35.91 ANISOU 1247 NE2 HIS 183 7.829 11.251 55.798 1.000 40.55 ANISOU 1247 NE2 HIS 183 7.829 11.251 55.798 1.000 40.55	ATOM 1221 O ANISOU 1221 CB ANISOU 1222 CB ANISOU 1223 CG ANISOU 1223 CG ANISOU 1224 SD ANISOU 1224 SD ANISOU 1225 CE ANISOU 1225 CE ANISOU 1225 CE ANISOU 1226 N ANISOU 1226 N ANISOU 1227 CA ANISOU 1227 CA ANISOU 1227 CA ANISOU 1228 C ANISOU 1228 C ANISOU 1228 C ANISOU 1229 O ANISOU 1229 O ANISOU 1229 O ANISOU 1230 CB ANISOU 1231 N ANISOU 1231 N ANISOU 1231 N ANISOU 1231 N ANISOU 1232 CA ANISOU 1232 CA ANISOU 1233 C ANISOU 1234 O ANISOU 1235 CB ANISOU 1236 CG ANISOU 1237 CD ANISOU 1237 CD	MET 180 7.629 MET 180 2377 MET 180 5.129 MET 180 5.339 MET 180 7280 MET 180 4.622 MET 180 4.622 MET 180 4.501 MET 180 6119 ALA 181 3523 ALA 181 3523 ALA 181 7.407 ALA 181 3980 ALA 181 2975 ALA 181 2903 ALA 181 4105 PRO 182 2782 PRO 182 10.442 PRO 182 2612 PRO 182 10.442 PRO 182 2612 PRO 182 10.448 PRO 182 2589 PRO 182 11.681 PRO 182 3352 PRO 182 10.215 PRO 182 3333	5064 7554 10.189 61.21 7966 8223 9.818 59.75 8911 7587 11.015 58.60 13510 7216 10.037 57.11 20000 4120 7.112 5646 6.140 60.98 3980 6250 6.591 3842 7.393 4765 4.817 4284 6.137 2296 4.817 4284 6.667 2870 2326 2491 2236 5.326 2759 3860 57.08 2486 2759 5.939 59.04 3582 3863 5.210 60.74	9 1.000 -452 7 1.000 -2331 8 1.000 4918 0 1.000 -1978 5 1.000 -625 7 1.000 -625 7 1.000 -32 7 1.000 -1023 0 1.000 -240 0 1.000 -335 8 1.000 -340 0 1.000 -391 0 1.	906 - 912 49.84 -1114 7 2 62.58 -3353 - 505 74.24 -262 - 905 79.59 1874 - 912 37.44 882 - 1132 37.40 2048 4 6 1 31.49 920 956 30.77 -98 164 42.66 1629 5 5 7 24.52 -76 3 2 0 20.55 -117 - 65 19.31 48 - 86 21.68 -340 - 55 24.98 -286 1 5 3 28.42 321 1 0 3 8
ATOM 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68	ANISOU 1239 CA ATOM 1240 C ANISOU 1241 C ATOM 1241 C ATOM 1242 CB ATOM 1242 CB ANISOU 1243 CG ANISOU 1243 CG ANISOU 1244 ND1 ANISOU 1244 ND1 ANISOU 1244 ND1 ATOM 1245 CD2 ANISOU 1245 CD2 ANISOU 1246 CE1 ANISOU 1247 NE2 ANISOU 1247 NE2	HIS 183 1882 HIS 183 10.749 HIS 183 1964 HIS 183 11.355 HIS 183 2297 HIS 183 8.338 HIS 183 1970 HIS 183 8.089 HIS 183 3100 HIS 183 7.884 HIS 183 4432 HIS 183 8.051 HIS 183 7.739 HIS 183 7.739 HIS 183 7.829 HIS 183 4375	2311 2652 8.124 54.33 1560 2456 9.061 54.86 2093 2504 7.781 54.83 2173 2945 9.120 55.44 2751 4281 9.362 56.80 4078 4926 10.311 54.82 2522 5898 10.658 56.98 4468 6565 11.251 55.79 3417 7614	-341 7 1.000 -75 8 1.000 -509 5 1.000 -136 7 1.000 -1190 1 1.000 1687 0 1.000 -472 8 1.000 1821	-455 3 4 6 15.74 -352 1 2 8 18.14 -127 - 1 3 5 18.66 -243 3 7 1 26.67 222 - 3 0 6 35.36 1466 - 1 4 5 4 33.00 -677 - 1 7 3 35.91 -625 - 2616 40.55 -1013 - 1590

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ANISOU			TYR		1717	1383	2916	-103	-443 150
ATOM ANISOU	1252		TYR		12.699	8.004	51.360		15.66
ANISOU	1252		TYR		1686	1323	2943	69 -3	66 -168
ANISOU	1253	CG	$ exttt{TYR}$		12.383	6.785 1313	50.562		14.85
MOTA			TYR		1743	5.540	2586	109	-567 4 3
ANISOU	1254	CD1	TYR		1549	1315	3021	-29	15.49 -575 190
ATOM	1255	CD2	TYR		12.329	6.836			15.89
ANISOU	1255	CD2	TYR	184	1724	1763	2552	55 -2	7 - 64
ATOM	1256	CE1	TYR		11.962	4.396		1.000	15.61
ANISOU ATOM	1256	CEL	TYR		1695	1244	2992	229	-137 1 1 3
ANISOU	1257	CE2	TYR	184	12.130 2340	5.661	48.447		17.52
ATOM	1258		TYR		11.915	1776 4.449	2540	4 83	- 9 0
ANISOU			TYR	184	1695	1736	3014	1.000 -156	16.96
ATOM	1259	OH	TYR		11.682	3.325		1 000	-480 3 4 18.81
ANISOU			TYR	184	2020	1775	3352	260	-277 - 312
ATOM	1260		ASP	185	10.924	10.330	50.502	1.000	14.36
ANISOU ATOM	1260		ASP	185	1518	1599	2338	87 -23	25 276
ANISOU			ASP ASP	185	10.026	11.005	49.574		
ATOM	1262		ASP	185 185	1875 10.240	1322	2078	141	-364 - 42
ANISOU	1262	Č	ASP	185	1182	10.490 1385	48.152 2211	-160	
ATOM	1263	0	ASP	185	11.357	10.135			-77 - 130
	1263		ASP	185	1177	1637	2559	-135	146 140
ATOM	1264	СВ	ASP	185	10.294	12.521	49.580	1.000	14.97
ANISOU ATOM	1264		ASP	185	1879	1293	2517	121	-186 - 159
ANISOU	1265		ASP ASP			13.155	50.830	1.000	
ATOM	1266			185 185	2680 9.507	1659 12.466	2351	232	-13 -172
ANISOU	1266	OD1	ASP		3553	3133	51.856 2314	443	
ATOM	1267	OD2	ASP		9.174	14.257	50.742		-302 5 2 1 24 3 2
	1267	OD2		185	4063	1730	3449	644	1140 - 16
ATOM	1268		LEU		9.141	10.465	47.382		12.57
ANISOU ATOM	1268 1269		LEU		1271	1378	2126	-117	-117 -117
	1269		LEU LEU		9.169 1533	10.091	45.986	1.000	12.92
ATOM	1270		LEU	186		1225 11.292	2150	-331	-84 -175
ANISOU	1270		LEU		1730	1307	45.052 2330	-93	-165 5 5
ATOM	1271		LEU		8.971	11.173	43.849		20 12
	1271		LEU	186	3721	1643	2280	-423	
ATOM	1272		LEU		8.040	9.106	45.609	1.000	
ANISOU ATOM	1272 1273		LEU		1509	1310	2393	-270	-375 - 6
ANISOU	1273	CG	LEU LEU	186	8.020 1549	7.811 1141	46.438		
ATOM	1274	CD1	LEU		6.929		3361 45.866	-145	-307 1 6 8
ANISOU	1274	CD1	LEU		1686	1845	3825	-700	-209 3 9 6
\mathtt{ATOM}	1275	CD2	LEU	186	9.369	7.115	46.341	1.000	18.32
ANISOU	1275	CD2		186	1689	1742	3528	200	-432 1 7 9
ATOM ANISOU	1276	N	SER	187	9.286	12.494	45.618		13.60
ATOM	1276 1277	C 2	SER		1326	1234	2608	-26	-95 137
ANISOU	1277	CA	SER SER		9.388 1489		44.826		
ATOM	1278		SER		10.736	1197 13.853	2338	- 54	-68 2 9 12.79
	1278	С	SER	187		1186	2192	-17	-114 - 9 O
ATOM	1279		SER	187	11.683	13.076	44.356	1.000	
ANISOU			SER	187	1532	1257	2720		24 - 113
MOTA	1280	CB	SER	187	9.201	14.915	45.811	1.000	12.87
ANISOU ATOM	1280		SER		1463	1282	2147	164	-154 9 8
ANISOU	1281	00	SER SER	187		14.873	46.716		13.22
		JG	SEK	187	1589	1420	2015	- 3 4	-143 2 2 4

ATOM 1282 N MET 188 10.898 14.844 43.292 1.000 13.44

ANISOU 1282 N MET 188 1552 1334 2221 -64 -34 - 26

ATOM 1283 CA MET 188 12.215 15.380 42.878 1.000 12.11

ANISOU 1283 CA MET 188 1508 1261 1833 29 -60 - 61

ATOM 1284 C MET 188 12.853 16.022 44.104 1.000 12.78

ANISOU 1284 C MET 188 1563 1156 2136 167 -311 - 42

ATOM 1285 O MET 188 13.896 15.550 44.600 1.000 13.40

ANISOU 1285 O MET 188 1408 1390 2294 116 -264 - 26

ATOM 1286 CB MET 188 12.038 16.300 41.667 1.000 13.66

ANISOU 1286 CB MET 188 1565 1501 2123 44 -161 207

ATOM 1287 CG MET 188 13.296 17.095 41.315 1.000 14.05

ANISOU 1287 CG MET 188 1697 1595 2046 66 150 1 3 3 - 55 -1287 CG MET 188 1697 1595 2046 66 150 1 3 3 1288 SD MET 188 14.600 15.971 40.752 1.000 14.96 ANISOU 1287 CG MET MOTA ATOM 1288 SD MET 188 1565 1591 2529 109 -81 1 1 0 ATOM 1289 CE MET 188 16.005 17.102 40.686 1.000 17.74 ANISOU 1289 CE MET 188 1852 2032 2855 -242 505 121 ATOM 1290 N VAL 189 12.244 17.112 44.616 1.000 12.62 ANISOU 1290 N VAL 189 1586 1203 2007 103 -147 -134 ATOM 1291 CA VAL 189 12.565 17.671 45.918 1.000 12.60 ANISOU 1291 CA VAL 189 1412 1438 1937 -228 -11 - 4 4 VAL 189 11.285 17.968 46.679 1.000 11.71 ATOM 1292 C ANISOU 1292 C VAL 189 1328 1294 1825 -170 -171 - 49 ATOM 1293 O VAL 189 10.227 18.099 46.050 1.000 12.56

ANISOU 1293 O VAL 189 1446 1291 2036 21 -320 -49

ATOM 1294 CB VAL 189 13.440 18.955 45.856 1.000 12.95

ANISOU 1294 CB VAL 189 1150 1517 2252 -174 -205 9 4

ATOM 1295 CG1 VAL 189 14.778 18.637 45.167 1.000 15.54

ANISOU 1295 CG1 VAL 189 1376 2094 2437 -140 161 9 1

ATOM 1296 CG2 VAL 189 1763 1391 2547 -130 -483 8 1

ATOM 1297 N THR 190 11.425 18.067 47.984 1.000 12.18

ANISOU 1297 N THR 190 1445 1422 1760 -109 -130 1 0

ATOM 1298 CA THR 190 10.353 18.454 48.897 1.000 11.98

ANISOU 1298 CA THR 190 10.879 19.630 49.710 1.000 12.47

ANISOU 1299 C THR 190 10.879 19.630 49.710 1.000 12.47

ANISOU 1299 C THR 190 11.959 19.523 50.320 1.000 15.06

ANISOU 1300 O THR 190 1424 1767 2531 46 -571 -446

ATOM 1301 CB THR 190 9.913 17.297 49.808 1.000 13.16

ANISOU 1302 OG1 THR 190 1693 1469 2334 -100 -25 -194

ATOM 1302 CG2 THR 190 1693 1469 2334 -100 -25 -194

ATOM 1303 CG2 THR 190 1693 1469 2334 -100 -25 -194 1293 O VAL 189 10.227 18.099 46.050 1.000 12.56 ATOM ATOM 1303 CG2 THR 190 8.778 17.723 50.734 1.000 14.79 ANISOU 1303 CG2 THR 190 1696 1510 2415 73 258 - 89 1304 N LEU 191 10.148 20.724 49.732 1.000 12.97 ATOM ANISOU 1304 N LEU 191 1329 1449 2149 23 -21 - 286 1305 CA LEU 191 10.511 21.908 50.526 1.000 13.75 ATOM ANISOU 1305 CA LEU 191 1543 1442 2238 78 -206 -301 ATOM 1306 C LEU 191 9.603 21.964 51.763 1.000 14.47 ANISOU 1306 C LEU 191 1543 1689 2265 83 -179 -412 ATOM 1307 O LEU 191 8.370 21.868 51.645 1.000 16.58 ANISOU 1307 O LEU 191 1517 2486 2297 219 -176 -725 ATOM 1308 CB LEU 191 10.398 23.212 49.722 1.000 15.37 ANISOU 1308 CB LEU 191 1717 1444 2680 58 -106 -189 ATOM 1309 CG LEU 191 11.705 23.578 48.973 1.000 16.10 ANISOU 1309 CG LEU 191 1747 1688 2680 -128 -113 -135 ATOM 1310 CD1 LEU 191 12.069 22.565 47.906 1.000 16.67 ANISOU 1310 CD1 LEU 191 2034 2093 2209 -23 -64 1 9 ATOM 1311 CD2 LEU 191 11.570 24.959 48.350 1.000 18.53 ANISOU 1311 CD2 LEU 191 2297 1906 2837 -345 -437 1 4 8 ILE 192 10.199 22.148 52.946 1.000 15.36 ATOM 1312 N

			PC1/GB98/03860
		- 56 -	
ANISOU 1312 N IL:	E 192 1479		_
ATOM 1313 CA TI.		2152	2204 -47 -165 - 164
ANISOU 1313 CA ILI		22.162	2 54.194 1.000 15 13
ATOM 1314 C IL	192 1450	2043	2251 -304 -173 - 280
331770000		23.423	55.010 1.000 15.58
3.00.00		1973	20-1-1-1-000 13.30
3377001		23.691	2251 -199 -254 -226 55.381 1.000 17.20
3 77 0 3 4 4 4 4	192 1856	2449	2.000 17.20
ATOM 1316 CB ILE	192 9.722	20.920	2229 -307 -341 -574
ANISOU 1316 CB ILE	192 2245	1958	2.000 17.03
ATOM 1317 CG1 ILE	1000	19.596	2266 -52 325 -303
ANISOU 1317 CG1 ILE	192 3040	2010	21227 21000 19.80
ATOM 1318 CG2 TTE	100 0 00		44/3 - 71 + 128 - 202
ANISOU 1318 CG2 ILE	192 2270	20.967	30.403 1.000 18.14
ATOM 1319 CD1 TLE	102 0 400	2354	4464 229 290 - 250
ANISOU 1319 CD1 TLE	192 4658	18.387	55.235 1.000 31 57
ATOM 1320 N GLM		2114	5222 -398 -1094 765
ANISOU 1320 N GLN	0.025	24.172	55.249 1.000 17.04
ATOM 1321 CA GLN		2185	2248 112 -388 - 301
7 17 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7		25.291	56.201 1.000 17.70
3 (10) (1200	, , , ,	2167	2824 -204 -186 -559
AMERICA 1222 C GLIN		24.869	2824 -204 -186 -559 57.443 1.000 19.67
30016 1305		2624	2969 -232 211 -840
ANT COLL 1222	193 7.082	23.942	2969 -232 211 -840
ANISOU 1323 O GLN ATOM 1324 CB GLN	193 2066	3843	57.426 1.000 26.60 4197 -965 -110.6 2
	193 8.129	26.598	4197 -965 -110 6 2
ANISOU 1324 CB GLN	193 3070	2388	55.643 1.000 23.74 3561 500 -98 -514
ATOM 1325 CG GLN	193 8.913	27.304	m
ANISOU 1325 CG GLN	193 4664	2384	54.559 1.000 28.26 3689 656 209 0
ATOM 1326 CD GLN	193-8.338	28.665	3689 656 209 0
ANISOU 1326 CD GLN	193 2868	2943	54.156 1.000 26.30
ATOM 1327 OE1 GLN	193 7.193	28.695	4181 791 3 111
ANISOU 1327 OE1 GLN	193 2826	7147	53.688 1.000 45.31
ATOM 1328 NF2 CIM	193 9.080	29.748	7241 -51 -616 3173
ANISOU 1328 NE2 GLN	193 3609	2588	54.345 1.000 30.44
ATOM 1329 N GLM		2588	5368 418 1259 692
ANISOU 1329 N GLN		25.259	58.645 1.000 22.04
ATOM 1330 CA GIM		2758	2090 303 -368 - 83
ANISOU 1330 CA GLN		24.793	59.847 1.000 22.68
ATOM 1331 C GIN		2617	2855 82 -230 -150
ANISOU 1331 C GLN		26.054	60.663 1.000 22.19
ATOM 1332 O GIN	101	2768	4856 117 -396 - 320
ANISOU 1332 O GLN		27.100	60.418 1.000 25.26
ATOM 1333 CB CIN		2877	26/9 -313 -31 411
ANISOU 1333 CB GLN		23.943	60.739 1.000 29 21
ATOM 1334 CG GLM		2101	3899 477 -50 939
ANISOU 1334 CG GIN		22.735	60.083 1.000 28 80
ATOM 1335 CD GIN	194 3108	3530	4305 576 -121 191
ANISOU 1335 CD GLN	194 10.296	22.332	60.962 1.000 31.97
ATOM 1336 OE1 GLN	194 2961	5384	3800 824 359 1075
ANISOU 1336 OE1 GLN		22.325	60.474 1.000 27.28
ATOM 1337 NE2 GLN		4189	3397 118 133 -249
ANISOU 1337 NE2 GLN	194 9.998	22.100	62.232 1.000 29.82
ATOM 1338 N THR	194 3540	3958	3832 989 645 800
ANT COTT 1222	195 6.419	25.891	61.658 1.000 23.30
3001	195 2407	3058	3387 -211 -235 - 720
AMEGOR TOO	195 6.476		3387 -211 -235 -720 62.768 1.000 27.14
300016 20.0	195 3459		3308 25 -50 - 890
33770011 1011	±95 6.933 3		3308
A COM A SA A	195 3825		3268 558 19 -1247
3377 0077 4345	195 6.639		
ANISOU 1341 O THR ATOM 1342 CB THR	195 2973		63.994 1.000 28.17 4815 481 171 -1030
ANTOON 1215 CD INK	195 5.149		
ANISOU 1342 CB THR			63.069 1.000 25.87
	2		3551 -16 -592 -1137

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- 57 -
                     1343 OG1 THR 195 4.111
   MOTA
                                                                                                26.550 63.196 1.000 25.45
   ANISOU 1343 OG1 THR 195 3427
3101
                                                                                                                         3141 -9 -117 - 750
                      1344 CG2 THR 195 4.788 28.396 61.847 1.000 31.31
                      1358 N ALA 198 5.771 25.791 70.866 1.000 37.27
  ANISOU 1358 N ALA 198 5038 4984 4139 -421 1647 -2070
ATOM 1359 CA ALA 198 5.983 26.811 71.888 1.000 35.91
  ANISOU 1359 CA ALA 198 6273 4144 3230 910 522 -1230
ATOM 1360 C ALA 198 6.993 26.328 72.921 1.000 44.30 ANISOU 1360 C ALA 198 5998 6138 4696 -193 -199 3 3 ANISOU 1361 O ALA 198 7.759 27.127 73.457 1.000 42.85 ANISOU 1361 O ALA 198 7.759 6328 4742 7 490 - 5.55 ATOM 1362 CB ALA 198 7.888 5697 23.55 10.00 41.70 ANISOU 1362 CB ALA 198 7.888 5697 23.55 10.00 41.70 ANISOU 1363 N ASN 199 7.036 25.036 73.225 1.000 34.93 ANISOU 1364 CA ASN 199 7.036 25.036 73.225 1.000 34.93 ANISOU 1364 CA ASN 199 7.969 24.578 74.264 1.000 33.58 ANISOU 1365 C ASN 199 9.352 24.262 73.718 1.000 31.53 ANISOU 1366 O ASN 199 4077 5048 2853 384 -420 - 85.5 ATOM 1366 O ASN 199 4077 5048 2853 384 -420 - 85.5 ATOM 1367 CB ASN 199 4077 5048 2853 384 -420 - 85.5 ATOM 1367 CB ASN 199 4533 5029 4262 859 584 - 5.2 2 ATOM 1368 CG ASN 199 4533 5029 4262 859 584 - 5.2 2 ATOM 1368 CG ASN 199 4030 4863 2993 882 202 1.78 ANISOU 1368 CG ASN 199 4030 4863 2993 882 202 1.78 ANISOU 1369 OD1 ASN 199 4030 4863 2993 882 202 1.78 ANISOU 1369 OD1 ASN 199 4030 4863 2993 882 202 1.78 ANISOU 1369 OD1 ASN 199 4030 4863 2993 882 202 1.78 ANISOU 1369 OD1 ASN 199 4030 4863 2993 882 202 1.78 ANISOU 1369 OD1 ASN 199 4030 4863 2993 882 202 1.78 ANISOU 1369 OD1 ASN 199 4030 4863 2993 882 202 1.78 ANISOU 1369 OD1 ASN 199 4030 4863 2993 882 202 1.78 ANISOU 1369 OD1 ASN 199 4030 4863 2993 882 202 1.78 ANISOU 1369 OD1 ASN 199 4030 4863 2993 882 202 1.78 ANISOU 1369 OD1 ASN 199 4030 4863 2993 882 202 1.78 ANISOU 1370 ND2 ASN 199 6.393 21.190 74.314 1.000 36.42 ANISOU 1370 ND2 ASN 199 3508 6251 4078 -13 1132 - 958 ANISOU 1370 ND2 ASN 199 3508 6251 4078 -13 1132 - 958 ANISOU 1370 ND2 ASN 199 3508 6251 4078 -13 1132 - 958 ANISOU 1370 ND2 ASN 199 3508 6251 4078 -13 1132 - 958 ANISOU 1371 N GLY 200 9.616 24.569 72.449 1.000 30.93
                      1360 C ALA 198 6.993 26.328 72.921 1.000 44.30
  ATOM
                       1371 N
                                               GLY
                                                               200 9.616 24.569 72.449 1.000 30.93
  ANISOU 1371 N
                                                GLY
                                                               200 4342
                                                                                                 4232
                                                                                                                        3179 436
                                                                                                                                                             144 - 692
                                                               200 10.920 24.304 71.866 1.000 35.26
                       1372 CA GLY
  ANISOU 1372 CA GLY
                                                                200 4430
                                                                                                 4905
                                                                                                                        4060 -317 480 -2400
  ATOM
                       1373 C
                                                GLY
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ANISOU 1373 C GLY 200 4683 4375 4936 -360 1601 -1460 ATOM 1374 O GLY 200 12.257 22.566 70.897 1.000 32.71 ANISOU 1374 O GLY 200 3921 4072 4436 -377 752 -1400 ATOM 1375 N PHE 201 10.264 21.939 71.588 1.000 28.666 ANISOU 1375 N PHE 201 3813 4229 2847 145 463 -326 ATOM 1376 CA PHE 201 10.491 20.575 71.106 1.000 27.55 ANISOU 1376 CA PHE 201 3190 4337 2943 -233 219 -672 ATOM 1377 C PHE 201 3190 4337 2943 -233 219 -672 ATOM 1377 C PHE 201 10.752 20.553 69.600 1.000 24.89 ANISOU 1378 O PHE 201 2943 3682 2832 190 -268 -379 ATOM 1378 O PHE 201 9.994 21.255 63.910 1.000 28.22 ANISOU 1378 O PHE 201 9.994 21.255 63.910 1.000 28.22 ANISOU 1379 CB PHE 201 9.250 19.729 71.413 1.000 30.46 ANISOU 1379 CB PHE 201 9.250 19.729 71.413 1.000 30.46 ANISOU 1379 CB PHE 201 9.250 19.729 71.413 1.000 30.46 ANISOU 1380 CG PHE 201 9.425 18.262 71.027 1.000 34.89 ANISOU 1380 CG PHE 201 4015 4609 4632 -772 162 8 9 ATOM 1381 CD1 PHE 201 10.395 17.472 71.605 1.000 31.18 ANISOU 1381 CD1 PHE 201 3436 4103 4310 -875 -93 -1105 - 58 -1382 CD2 PHE ANISOU 1382 CD2 PHE 1383 CE1 PHE 201 6489 3608 4239 -1078 -1475 -500 201 8.761 16.363 69.679 1.000 31.78 201 4327 3911 3838 652 250 1 1 9 201 9.755 15.606 70.265 1.000 29.78 201 3705 3397 4211 6 -638 -849 ANISOU 1383 CE1 PHE ATOM 1384 CE2 PHE ANISOU 1384 CE2 PHE MOTA 1385 CZ PHE ANISOU 1385 CZ PHE MOTA 1386 N VAL 202 11.706 19.751 69.144 1.000 23.51 ANISOU 1386 N 202 2671 3392 VAL 2868 -292 -1 -578 ATOM 1387 CA VAL 202311.969 19.626 67.706 1.000 26.37 ANISOU 1387 CA VAL 202 3025 4050 2946 -667 57 -724 MOTA 1388 C VAL 202 11.423 18.283 67.198 1.000 22.75 ANISOU 1388 C VAL 202 2729 3348 2567 96 -120 -435 1389 0 VAL 202 11.880 17.190 67.541 1.000 28.71 202 3249 3799 3859 119 31 66 3 202 13.476 19.721 67.415 1.000 24.99 202 3060 3427 3008 -278 283 1 202 13.715 19.464 65.938 1.000 27.70 ANISOU 1389 O VAL 119 31 661 ATOM 1390 CB VAL ANISOU 1390 CB VAL 3008 -278 283 152 1391 CG1 VAL ATOM ANISOU 1391 CG1 VAL 202 4642 2577 3307 87 1014 - 3 202 14.050 21.071 67.823 1.000 26.80 1392 CG2 VAL MOTA ANISOU 1392 CG2 VAL 202 2826 3868 3487 -490 474 -1 203 10.405 18.402 66.333 1.000 24.10 -490 474 -398 ATOM 1393 N SER 203 2194 3607 203 9.634 17.231 203 2373 3584 ANISOU 1393 N 3607 3356 -31 -179 -528 17.231 65.940 1.000 23.70 SER 1394 CA SER ATOM ANISOU 1394 CA SER 203 2373 3584 3046 -290 308 -203 10.168 16.511 64.710 1.000 21.28 -290 308 -533 1395 C ATOM SER ANISOU 1395 C 203 2173 SER 3041 2871 46 227 - 42 203 10.159 15.285 64.640 1.000 27.60 1396 0 MOTA SER 1010 - 249 203 - 2064 1099 - 382 1399 N ATOM LEU 204 10.688 17.233 63.724 1.000 22.46 ANISOU 1399 N LEU 204 2476 3013 3043 79 450 - 46 ATOM 1400 CA LEU ANISOU 1400 CA LEU 204 2200 2831 2667 45 -18 - 15 ATOM 1401 C 204 12.595 16.038 62.747 1.000 18.83 LEU ANISOU 1401 C LEU 204 2151 2528 2477 -75 60 - 1ATOM 1402 O LEU 204 13.443 16.783 63.251 1.000 20.47 ANISOU 1402 O LEU 204 2333 2386 3059 -303 -195 4 0 4 1403 CB LEU ATOM 204 11.103 17.486 61.362 1.000 21.42 ANISOU 1403 CB LEU 204 2718 2548 2871 311 -16 - 8

10.188 61.079 1.000 33.57 4319 5617 177 -1316 18.747 59.660 1.000 36.19 3807 5540 1276 -1167 17.234 61 210 1404 CG LEU 204 9.769 18.183 61.079 1.000 33.57 ATOM 204 2820 ANISOU 1404 CG LEU -1316 1172 1405 CD1 LEU 204 9.797 ANISOU 1405 CD1 LEU 204 4402 5540 1276 -1167 987 1406 CD2 LEU 204 8.581 204 3058 5328 5960 -526 -1896 205 12.864 14.836 62.284 1.000 20.33 ANISOU 1406 CD2 LEU -526 -1896 686 1407 N GLN ANISOU 1407 N 205 2518 GLN 2563 2644 104 -31 -129 205 14.209 14.247 1408 CA GLN62.335 1.000 18.88 ANISOU 1408 CA GLN 205 2522 2225 2425 -6 -181 3 6 205 14.512 13.504 61.036 1.000 18.19 1409 C MOTA GLN ANISOU 1409 C 205 1986. GLN 2383 2543 -143 -188 - 80 205 13.577 13.033 60.408 1.000 19.87 1410 0 MOTAGLN ANISOU 1410 O 205 1974 3063 GLN -125 -212 -237 2514 1411 CB GLN 205 14.296 13.267 63.493 1.000 24.25 MOTA ANISOU 1411 CB GLN 205 3948 2716 2548 202 -343 2 9 6 1412 CG GLN ATOM 205 14.164 13.948 64.856 1.000 30.64 ANISOU 1412 CG GLN 205 4099 5159 2382 850 -327 - 89MOTA 1413 CD GLN 205 14.744 13.078 65.948 1.000 28.28 ANISOU 1413 CD GLN 205 4473 3633 2640 -161 -1015 -390 1414 OE1 GLN 205 14.307 11.921 66.041 1.000 37.69 ANISOU 1414 OE1 GLN 205 5733 5073 3515 -2145 -699 4 7 8 ATOM 1415 NE2 GLN 205 15.710 13.553 66.711 1.000 40.53

ANISOU 1415 NE2 GLN 205 6798 4417 4185 -1341 -2865 3 2 3

ATOM 1416 N ALA 206 15.752 13.471 60.576 1.000 18.52

ANISOU 1416 N ALA 206 2070 2199 2769 -240 -13 4

ATOM 1417 CA ALA 206 16.152 12.700 59.405 1.000 18.42

ANISOU 1417 CA ALA 206 2074 2351 2575 -100 -158 2 3

ATOM 1418 C ALA 206 2074 2351 2575 -100 -158 2 3

ATOM 1418 C ALA 206 17.343 11.802 59.738 1.000 17.41

ANISOU 1418 C ALA 206 2107 2158 2350 -185 -254 - 1 7

ATOM 1419 O ALA 206 18.123 12.203 60.613 1.000 20.67

ANISOU 1419 O ALA 206 2469 2410 2973 -48 -711 - 3 9 6

ATOM 1420 CB ALA 206 16.637 13.599 58.270 1.000 18.77

ANISOU 1420 CB ALA 206 2119 2310 2703 156 -65 1 4 7

ATOM 1421 N GLU 207 17.492 10.764 58.931 1.000 18.09

ANISOU 1421 N GLU 207 2092 2101 2680 -249 -496 -162 1415 NE2 GLN 205 15.710 13.553 66.711 1.000 40.53 ATOM ATOM 207 18.710 9.944 1422 CA GLU ANISOU 1422 CA GLU 207 2210 207 19.851 10.730 58.320 1.000 19.98 ATOM 1423 C GLU ANISOU 1423 C 207 2018 2233 GLU 3342 220 -560 5 4 4 GLU 207 19.732 11.068 57.143 1.000 20.33 MOTA GLU 207 19./32 11.13 GLU 207 2000 2753 2970 5 -4/1 5 207 19 566 8.623 58.214 1.000 24.03 1424 0 ANISOU 1424 O 1425 CB GLU 207 18.566 8.623 ATOM ANISOU 1425 CB GLU 207 3401 1784 3946 316 -1226 6 1 ATOM 1426 CG GLU 207 19.757 7.674 58.295 1.000 24.35 ANISCU 1426 CG GLU 207 3223 1907 4121 354 93 4 6 7 1427 CD GLU 207 20.730 7.791 57.129 1.000 31.69 MOTA ANISOU 1427 CD GLU 207 2729 5178 4134 -1218 -175 1 2 2 1428 OE1 GLU 207 20.376 7.611 55.943 1.000 26.97 ATOM ANISOU 1428 OE1 GLU 207 2849 3404 ATOM 1429 OE2 GLU 207 21.908 8.121 3993 31 -256 309 57.407 1.000 30.70 ANISOU 1429 OE2 GLU 207 2484 3416 5764 -233 -342 -1168 ATOM 1430 N VAL 208 20.919 10.936 59.078 1.000 18.53 ANISOU 1430 N VAL 208 2020 2112 2907 130 -362 3 2 0 ATOM 1431 CA VAL 208 22.150 11.547 58.541 1.000 19.53 AMISOU 1431 CA VAL 208 2044 2238 3137 39 -476 630 ATOM 1432 C VAL 208 23.341 10.755 59.088 1.000 21.95 ANISOU 1432 C VAL 208 2040 2792 3507 225 -461 7 9 7 1433 0 ATOM VAL 208 23.460 10.663 60.314 1.000 23.82 ANISOU 1433 O VAL 208 2262 3240 3547 -40 -858 8 2 5 1434 CB VAL ATOM 208 22.271 13.027 58.905 1.000 19.72

	PC1/GB98/03860
ANTCOLLAGA	- 60 -
ANISOU 1434 CB VAL 208 1918 ATOM 1435 CG1 VAL 208 208	2429 3145 -47 -308 3 1 1
3NI CON 1135 CC1 VRL 208 23.52	2429 3145 -47 -308 3 1 1 24 13.626 58.281 1.000 23.14
ANISOU 1435 CG1 VAL 208 23.52 ATOM 1436 CG2 VAL 208 2524	2374
NTCOV 1100 CG2 VAL 208 21.03	3895 -202 284 3 4 9 13.812 58.469 1.000 19.47
	2279 2650 272
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3 more 1 4 3 5	2449 4122 465
ANTECOT 110 011 011 209 25.30	6 9.374 58.773 1.000 26.42
3004 1430	2222 44504 460 402
33770077 1100	5 8.250 59.695 1.000 30.01
3 00 1 2 1 2 2 2 3 3 4 0 3	3240
209 25.60	9 7.835 60 629 1 000 31^{-2}
7 TOM 1442 200 4000	3418 100E 007 0 n
ANTEGOTE 1441 210 43.09	1 7.702 59.523 1 000 26 64
7 TOM 1440 = 210 3103	_ 3214 3/44 259 -85 350
7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	3 6.585 60.360 1.000 29 78
ATOM 1443 C GLV 210 22 62	_ 3019 -55 -997 5 g A
ANISOU 1443 C GLY 210 5227	2 6.993 61 663 1 000 20 20
ATOM 1444 O GLV 210 22 16	_ *212
ANISOU 1444 O GLV 210 4152	0.18/ 62.481 1.000 41 45
ATOM 1445 N ALA 211 22	-1874 - 5082 - 1874 - 567 2316
ANISOU 1445 N ALA 211 4903	61.976 1.000 32.81
ATOM 1446 CA ATA 211 21 22	$\frac{4023}{303}$ 303/ 1372 -1177 632
ANISOU 1446 CA ALA 211 3002	5050 63.235 1.000 35.62
144/(ATA 211 20 cc-	3584 1061 -610970
	4737
1448 () AT.A 011 00 ccc	
ATOM 1448 U ALA 211 3661	4062 3020 574
ANTCOM 1449 CB ALA 211 22.812	
200 1449 CB ALA 211 3644	8904 3160 1.000 41.36
ANT CON 1450 1116 212 19.682	3169 1372 -18 -791 9.676 63.825 1.000 36.68
7 TOM 1451 212 3211	4237 4480 1166 1000
ANT CON 115 212 18.620	423/ 4489 1166 1265 2171 10.654 63.641 1.000 28.82
7 m o x 2 4 m = 2 m o x 2 m o	3167 3293 263 504 1027
NITCOL 1100	12.023 64.124 1 000 34 72
ATOM 1453 0 PHP 312 10	3/60 4685 -248 -53 0 77 c
ANT CON 1 4 4 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	12.191 65 210 1 000 30 12
ATOM 1454 CB PHR 212 17 27	3335 -549 -1129 1220
ANISOU 1454 CB PHE 212 6376	10.219 64.388 1.000 45.35
ATOM 1455 N THP 212 10	2309 8288 1348 3748 2314
ANISOU 1455 N THR 213 4134	2720 63.271 1.000 26.30
ATOM 1456 CA THE 212 10	2/30 3122 662 -581 1 0 0
THR 213 TEST	2052
ANTEGOT 145/ C THR 213 18.190	
THR 213 2835	2652
ANT COT 1458 0 THR 213 17.329	
ATOM 1450 U THR 213 2640	2222 2.000 21.40
ANT COT: 1455 32 1111 213 20.398	2269 3223 -328 -580 -179 14.759 62.308 1.000 27.60
3 m O M	3330
ANTCON 1466 551 1RR 213 21.673	3220 4113 189 -356 - 798 14.084 62.374 1.000 32.00
	4220 4356 746 -410 5 2 0
MITCON 1462 THR 213 20.735	16.254 62.355 1 000 20 45
ATOM 1462 N ASP 214 10 11	3320 3448 -106 -1265 -204
ANT COV. 1450.119	16.177 64.371 1.000 21 05
ATOM 1463 CA ASP 214 17 200	2236 2972 -82 -380 - 142
ANISOU 1463 CA ASP 214 2742	17.110 64.462 1.000 20.61
ATOM 1464 C ASP 214 162	2095 2993 -117 -898 - 37g
ANISOU 1464 C ASP 214 2373	18.030 63.226 1.000 20.58
214 23/3	2525 2923 182 -169 - 237
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ATOM
         1465 C
                   ASP
                         214 18.018 18.430 62.678 1.000 23.02
ANISOU 1465 O
                    ASP
                          214 2461
                                        2883
                                                   3404
                                                           -167 -52 -572
MOTA
         1466 CB
                   ASP
                          214 17.205 18.058 65.637 1.000 23.54
ANISOU 1466 CB
                   ASP
                          214 3304
                                        2607
                                                   3032
                                                           -92
                                                                   -748 - 668
MOTA
         1467 CG
                   ASP
                          214 16.915 17.506 67.004 1.000 24.93
ANISOU 1467 CG
                                        2850
                   ASP
                          214 3545
                                                   3079
                                                           450
                                                                   -417 -614
         1468 OD1 ASP
ATOM
                          214 16.357 16.395 67.113 1.000 29.17
ANISOU 1468 OD1 ASP
                         214 4134 3070 3878 202 -705 2
214 17.276 18.191 67.990 1.000 34.38
                                                                   -705 2 6 2
        1469 OD2 ASP
ANISOU 1469 OD2 ASP
                                        3040
                          214 6917
                                                   3107
                                                          1017 -1413 -736
         1470 N
                         215 15.802 18.452 62.859 1.000 20.74
                   LEU
ANISOU 1470 N
                   LEU
                         215 2426
                                         2372
                                                   3081
                                                           86 -60 3 0 6
                         215 15.568 19.401 61.796 1.000 20.55
        1471 CA
                   LEU
ANISOU 1471 CA
                   LEU
                         215 2895
                                         2013
                                                   2899
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                         215 14.724 20.552 62.332 1.000 19.02
ATOM
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                   LEU
ANISOU 1472 C
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ANISOU 1473 O
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ANISOU 1481 O
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ATOM
ANISOU 1482 CB
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ATOM
        1483 CG
                  PRO
ANISOU 1483 CG
                   PRO
ATOM
        1484 CD
                  PRO
ANISOU 1484 CD
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ATOM
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30001	/ / / /	6483 -1462 -545 1 6 6
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ATOM 1499 C ARG	218 14.113 29.33	4419 - 784 - 1349 269
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ATOM 1500 O ARG	218 13.746 29.17	4910 -180 -000 cc
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ATOM 1503 CD ARC		0010 -3031 430 100
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ATOM 1504 NE ARC		3484 -3596 -1165 1649
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ATOM 1507 NH2 NDC		4U/⊥ -1943 -1333 570
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ANISOU 1508 N PRO		00.972 1.000 25.89
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ANISOU 1509 CA PRO	219 2828 3120	00.326 1.000 28.10
ATOM 1510 C PRO	219 13.636 31.959	4/30 -410 379 -696
ANISOU 1510 C PRO	219 3141 3010	1.000 20.43
ATOM 1511 O PRO	219 12.904 32.393	4053 -190 116 -320
ANISOU 1511 O PRO	219 4734 3500	38.081 1.000 34.17
ATOM 1512 CB PRO	219 13.115 32.717	4750 302 -798 - 893
ANISOU 1512 CB PRO	219 5621 3612	5050 2.000 39.70
ATOM 1513 CG PRO	219 13.368 32.033	5852 -500 1615 -1527
ANISOU 1513 CG PRO ATOM 1514 CD PRO	219 6139 5277	62.628 1.000 42.38
	219 14.370 30.943	4688 -257 2084 -2086
ANISOU 1514 CD PRO ATOM 1515 N ASP	219 3901 5719	62.289 1.000 32.77 2831 -602 828 -1603
AMICOU 1515 N ASP	220 14.950 31 824	2831 -602 828 -1603
ATOM 1515 N ASP	220 3328 1582	58.811 1.000 25.65 4837 -276 801 -878
ANTICOT 1510 CE ASP	220 15.590 32 200	4837 -276 801 -878
ATOM 1518 CA ASP	220 3594 2115	57.587 1.000 26.45 4341 -782 248 -861
ANTCOU 1517 C ASP	220 15.781 31 305	4341 -782 248 -861
ΔTOM	440 3549 1843	56.451 1.000 28.46 5423 -111 1638 -942
ANT COLL 1515	420 16.432 31 620	5423 -111 1638 - 943
ATOM 1510	440 3249 2021	55.433 1.000 25.80 4533 -140 623 -412
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	440 2653 3531	9912 -812 230 -957
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ANTCOU : COS	221 15.292 30.072	6969 93 -824 -1266 56.537 1.000 24.79
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ANTCOM 1504 - ALA	221 15.695 29.016	3398 -252 671 -659 55.596 1.000 19.17
ATOM 1707 -	221 2165 1868	3251 -52 -92 -610
AMICOU 1505 - AMA	221 14.551 27.996	55.479 1.000 18.60
AN1500 1525 C ALA 2	221 1920 2238	2908 -82 -207 - 3.6.2
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- 63 -1526 0 ALA 221 13.763 27.852 56.415 1.000 26.47 ALA 221 4127 2641 3289 -1307 894 ANISOU 1526 O ALA 221 4127 2641 3289 -1307 894 -904 221 16.939 28.316 56.104 1.000 19.36 1527 CB ALA MOTA

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 ANISOU 1527 CB ALA ATOM 1528 N .VAL ANISOU 1528 N VAL ATOM 1529 CA VAL ANISOU 1529 CA VAL ATOM 1530 C VAL ANISOU 1530 C VAL 1531 0 VAL 222 1658 1730 3390 -108 -194 4 8 222 12.822 26.433 52.747 1.000 19.60 ANISOU 1531 O VAL 1532 CB VAL 1532 CB VAL 222 2267 2202 2979 91 -666 -304 1533 CG1 VAL 222 13.781 26.363 51.563 1.000 21.96 ANISOU 1532 CB VAL 1533 CG1 VAL 222 2252 3113 2977 250 -645 - 1534 CG2 VAL 222 11.730 25.411 52.490 1.000 22.44 ANISOU 1533 CG1 VAL 222 2252 2977 250 -645 -182 ATOM ANISOU 1534 CG2 VAL 222 2923 2537 3067 -497 -898 4 ATOM 1535 N LEU 223 13.789 23.892 54.621 1.000 16.30 3067 -497 -898 4 4 ANISOU 1535 N 1535 N LEU 223 1792 1694 2706 -239 -93 -1536 CA LEU 223 14.407 22.575 54.579 1.000 15.91 2706 -239 -93 -532 MOTA ANISOU 1536 CA LEU 223 1679 1864 2503 -93 -297 -333 LEU 223 14.114 21.908 53.243 1.000 14.86 ATOM . 1537 C ANISOU 1537 C LEU 223 1337 1537 2773 -141 -322 -458 LEU 223 12.969 21.888 52.766 1.000 16.23 MOTA 1538 O ANISOU 1538 O LEU 223 1317 2132 2719 70 -391 -281 1539 CB LEU 1539 CB LEU 1540 CG LEU 1540 CG LEU 1541 CD1 LEU MOTA 223 13.829 21.779 55.761 1.000 19.97 ANISOU 1539 CB 223:2740 1945 2901 -121 205 -2.12ATOM 223 14.298 20.348 55.882 1.000 23.01 ANISOU 1540 CG 223 2668 1871 4205 -375 -170 9 223 15.797 20.322 56.143 1.000 23.73 223 2570 3067 3378 69 135 3 1 6 -375 -170 9 1 АТОМ ANISOU 1541 CD1 LEU 223 13.492 19.668 56.979 1.000 35.71 223 2813 3296 7459 525 1116 2 224 15.115 21.370 52.570 1.000 14.18 1542 CD2 LEU ATOM ANISOU 1542 CD2 LEU 1116 2333 ATOM 1543 N VAL ANISOU 1543 N VAL 224 1383 1446 2560 -28 -320 - 205 1544 CA VAL 224 14.956 20.627 51.330 1.000 14.52 ANISOU 1544 CA VAL 224 1585 1501 2431 -23 -323 -127 ATOM 1545 C VAL 224 15.320 19.160 51.561 1.000 13.59 ANISOU 1545 C VAL 224 1464 1522 2178 23 -290 -251 1546 O VAL 224 16.442 18.861 51.981 1.000 15.38 ATOM ANISOU 1546 O VAL 224 1464 1558 2822 0 -505 -374 ATOM 1547 CB VAL 224 15.832 21.209 50.222 1.000 14.25 ANISOU 1547 CB VAL 224 1402 1606 2407 -60 -461 - 1081548 CG1 VAL ATOM 224 15.685 20.443 48.906 1.000 16.63 ANISOU 1548 CG1 VAL 224 1682 2474 -159 -408 - 421 2164 1549 CG2 VAL 224 15.575 22.687 50.040 1.000 16.40 ANISOU 1549 CG2 VAL 224 1807 1562 2863 6 -509 8 7 1550 N PHE 225 14.340 18.299 51.299 1.000 13.49 ANISOU 1550 N PHE 225 1494 1526 2106 -66 -353 - 130 ATOM 1551 CA PHE ANISOU 1551 CA PHE 225 14.647 16.882 51.162 1.000 14.67 225 1639 1505 2431 -115 -61 -283 ATOM 1552 C PHE 225 14.756 16.533 49.675 1.000 14.27 ANISOU 1552 C PHE 225 1536 1533 -260 - 194 2352 100 ATOM 1553 0 PHE 225 13.858 16.876 48.893 1.000 16.25 ANISOU 1553 O PHE 225 1604 2000 2569 296 -311 - 88 1554 CB PHE ATOM 225 13.537 15.999 51.749 1.000 15.57 ANISOU 1554 CB PHE 225 1613 1563 2740 -25 -46 2 4 MOTA 1555 CG PHE 225 13.387 15.996 53.257 1.000 17.95 ANISOU 1555 CG PHE 225 1888 2267 2666 -650 -302 2 0 3 1556 CD1 PHE ATOM 225 14.409 15.809 54.157 1.000 27.39

- 64 -ANISOU 1556 CD1 PHE 225 2740 4234 3431 -910 -1094 ATOM 1557 CD2 PHE 225 12.125 15.863 53.820 1.000 21.09 -910 -1094 900 225 2333 2765 2917 ATOM 1558 CE1 PHE 225 14.211 15.673 55.521 1.000 26.82

ATOM 1559 CE2 PHE 225 3108 3657 3424 -1044 -1241 112

ANISOU 1559 CE2 PHE 225 11.910 15.910 55.186 1.000 21.65

ATOM 1560 CZ PHE 225 2994 2414 2817 623 239 - 39

ANISOU 1560 CZ PHE 225 3705 3716 3531 -832 -663 340

ATOM 1561 N CYS 226 15.795 15.817 49.266 1.000 12.77

ANISOU 1561 N CYS 226 1428 1292 2131 -60 -370 - 239

ANISOU 1562 CA CYS 226 15.810 15.180 47.956 1.000 12.99

ATOM 1563 C CYS 226 14.903 13.956 47.985 1.000 12.37

ANISOU 1563 C CYS 226 14.903 13.956 47.985 1.000 12.37

ATOM 1564 O CYS 226 14.961 13.217 48.974 1.000 15.68

ANISOU 1565 CB CYS 226 17.228 14.855 47.527 1.000 13.77

ANISOU 1566 SG CYS 226 1410 1627 2193 19 -203 -75

ATOM 1566 SG CYS 226 1885 47.527 1.000 13.77

ATOM 1566 SG CYS 226 1410 1627 2193 19 -203 -75

ATOM 1566 SG CYS 226 1882 47.527 1.000 13.77 -166 399 -527 1558 CE1 PHE 225 14.211 15.673 55.521 1.000 26.82 -1044 -1241 1128 CYS 226 1410 1627 2193 19 -203 - 75 CYS 226 18.224 16.367 47.314 1.000 16.37 ATOM 1566 SG CYS 226 18.224 16.367 47.314 1.000 16.37

ANISOU 1566 SG CYS 226 1744 1740 2735 -222 -236 - 1 2

ANISOU 1567 N GLY 227 14.150 13.722 46.928 1.000 13.20

ANISOU 1567 N GLY 227 1388 1513 2113 -28 -293 - 2 9 0

ANISOU 1568 CA GLY 227 13.352 12.496 46.899 1.000 12.58

ATOM 1569 C GLY 227 1279 1631 1872 -83 -438 - 2 5 5

ANISOU 1569 C GLY 227 13.903 11.541 45.849 1.000 12.54

ANISOU 1569 C GLY 227 1518 1279 1965 15 -288 - 7 9

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ANISOU 1570 O GLY 227 1630 1523 2008 51 -155 8 2 227 1630 1523 2008 51 -155 8 2 228 13.212 10.400 45.712 1.000 13.02 ATOM 1571 N ALA ANISOU 1571 N ALA 228 1490 1306 2151 59 -204 -16 228 13.663 9.321 44.860 1.000 12.41 59 -204 - 161 ATOM 1572 CA ALA ANISOU 1572 CA ALA 228 1649 1155 1912 -68 -119 -9.727 43.404 1.000 12.82 -68 -119 - 63 1573 C ALA 228 13.706 9.727 MOTA ANISOU 1573 C ALA 228 1566 1288 2016 97 -223 - 5 ATOM 1574 O ALA 228 14.482 9.132 42.651 1.000 13.64 ANISOU 1574 O ALA 228 1717 1462 2004 26 -6 -131 ANISOU 1575 CB ALA 228 12.714 8.121 45.058 1.000 14.56 228 1808 1366 2356 -219 358 -243 1576 N 229 12.909 10.695 42.952 1.000 13.61 ILE

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 -289 2 7 3

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 ANISOU 1576 N ILE ATOM 1577 CA ILE ANISOU 1577 CA ILE ATOM 1578 C ILE ANISOU 1578 C ILE ATOM 1579 O ILE ANISOU 1579 O ILE . 1580 CB ILE 229 1470 1631 2015 171 -354 - 4 2 229 10.599 10.920 40.973 1.000 15.72 ANISOU 1580 CB ILE 1581 CG1 ILE 229 1218 1936 2817 85 31 1 1 8 229 12.040 12.674 39.808 1.000 14.19 229 1670 1425 2298 76 -364 1 7 2 229 10.745 9.924 39.836 1.000 20.03 ANISOU 1581 CG1 ILE 1582 CG2 ILE ATOM ANISOU 1582 CG2 ILE 76 - 364 174 ATOM 1583 CD1 ILE ANISOU 1583 CD1 ILE 229 2129 1814 3667 -208 -385 -488 ATOM 1584 N ALA 230 14.877 12.575 42.353 1.000 13.38 39.836 1.000 20.03 ANISOU 1584 N ALA 230 1252 1378 2454 -97 -176 7 4
ANISOU 1585 CA ALA 230 16.209 13.185 42.130 1.000 12.30
ATOM 1585 CA ALA 230 1156 1444 2074 66 -97 -1 08
ANISOU 1586 C ALA 230 17.223 12.033 41.976 1.000 12.89
ANISOU 1586 C ALA 230 1491 1327 2079 128 30 - 20

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- 65 -
                   ATOM 1587 O ALA 230 18.100 12.091 41.146 1.000 13.65 ANISOU 1587 O ALA 230 1240 1530 2418 108 4 4 6 ATOM 1588 CB ALA 230 16.588 14.000 43.345 1.000 13.66 ANISOU 1588 CB ALA 230 1559 1415 2215 -186 -21 -2 ATOM 1589 N THR 231 17.143 10.978 42.805 1.000 13.31
               ATOM 1589 N THR 231 17.143 10.978 42.805 1.000 13.31 ANISOU 1589 N THR 231 1526 1318 2214 58 -261 - 1 ATOM 1590 CA THR 231 18.022 9.815 42.659 1.000 13.32 ANISOU 1590 CA THR 231 1660 1307 2093 78 -302 3 2 ATOM 1591 C THR 231 17.906 9.224 41.251 1.000 13.32 ATOM 1592 O THR 231 18.932 8.974 40.620 1.000 15.51 ANISOU 1592 O THR 231 1468 1759 2667 245 58 -170 ANISOU 1593 CB THR 231 17.656 8.751 43.688 1.000 13.03 ANISOU 1593 CB THR 231 17.656 8.751 43.688 1.000 13.03 ANISOU 1593 CB THR 231 17.530 9.313 44.995 1.000 14.70 ATOM 1594 OG1 THR 231 17.530 9.313 44.995 1.000 14.70 ANISOU 1595 CG2 THR 231 17.530 9.313 44.995 1.000 14.70 ANISOU 1595 CG2 THR 231 18.698 7.621 43.697 1.000 13.69 ANISOU 1595 CG2 THR 231 18.698 7.621 43.697 1.000 13.69 ANISOU 1595 CG2 THR 231 1449 1419 2335 113 -211 197 ATOM 1596 N LEU 232 16.665 9.049 40.796 1.000 13.43 ANISOU 1597 CA LEU 232 16.446 8.396 39.527 1.000 14.11 ANISOU 1597 CA LEU 232 16.446 8.396 39.527 1.000 14.11 ANISOU 1597 CA LEU 232 16.446 8.396 39.527 1.000 14.11 ANISOU 1597 CA LEU 232 16.975 9.248 38.381 1.000 15.53
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ATOM 1597 CA LEU 232 16.446 8.396 39.527 1.000 14.11 ANISOU 1597 CA LEU 232 1809 1226 2326 80 -468 4 9 ANISOU 1598 C LEU 232 16.975 9.248 38.381 1.000 15.53 ANISOU 1598 C LEU 232 1968 1557 2376 209 -3 9 0 ANISOU 1599 O LEU 232 17.749 8.808 37.504 1.000 17.16 ANISOU 1600 CB LEU 232 14.940 8.135 39.368 1.000 14.47 ANISOU 1600 CB LEU 232 14.940 8.135 39.368 1.000 14.47 ANISOU 1601 CG LEU 232 1692 1630 2175 72 -396 -161 ANISOU 1601 CG LEU 232 194.525 7.307 38.155 1.000 15.89 ANISOU 1601 CG LEU 232 1941 1768 2329 120 -470 -303 ANISOU 1602 CD1 LEU 232 15.118 5.920 38.202 1.000 23.19 ANISOU 1603 CD2 LEU 232 15.118 5.920 38.202 1.000 23.19 ANISOU 1603 CD2 LEU 232 13.003 7.190 38.126 1.000 19.46 ANISOU 1603 CD2 LEU 232 2006 2262 3126 -470 -523 -66 ANISOU 1604 N VAL 233 16.539 10.514 38.299 1.000 19.46 ANISOU 1605 CA VAL 233 16.893 11.317 37.117 1.000 13.84 ANISOU 1605 CA VAL 233 16.893 11.317 37.117 1.000 13.84 ANISOU 1605 CA VAL 233 16.893 11.317 37.117 1.000 13.84 ANISOU 1606 C VAL 233 18.407 11.510 37.025 1.000 14.08 ANISOU 1606 C VAL 233 18.407 11.550 37.025 1.000 14.08 ANISOU 1606 C VAL 233 19.30 17.16 1658 1926 141 -73 10 7 ANISOU 1606 C VAL 233 193 12.30 17.000 13.84 ANISOU 1606 C VAL 233 18.940 11.587 35.910 1.000 14.08 ANISOU 1606 C VAL 233 18.940 11.587 35.910 1.000 14.08 ANISOU 1606 C VAL 233 18.940 11.587 35.910 1.000 14.08 ANISOU 1606 C VAL 233 16.098 12.626 37.062 1.000 14.08 ANISOU 1609 CG1 VAL 233 16.599 13.650 38.113 1.000 15.70 ANISOU 1600 CG2 VAL 233 16.599 13.650 38.113 1.000 15.70 ANISOU 1600 CG2 VAL 233 16.599 13.650 38.113 1.000 15.70 ANISOU 1610 CG2 VAL 233 16.599 13.650 38.113 1.000 15.70 ANISOU 1610 CG2 VAL 233 16.599 13.650 38.113 1.000 15.70 ANISOU 1610 CG2 VAL 233 16.599 13.650 38.113 1.000 15.70 ANISOU 1610 CG2 VAL 233 16.91 17.94 2083 146 -110 2 3 5 ANISOU 1610 CG2 VAL 233 16.91 17.94 2083 146 -110 2 3 5 ANISOU 1610 CG2 VAL 233 16.91 17.94 2083 146 -110 2 3 5 ANISOU 1610 CG2 VAL 233 16.91 17.94 2083 146 -110 2 3 5 ANISOU 1610 CG2 VAL 233 16.90 17.94 2083 146 -110 2 3 5 ANISOU 1610 CG2 VAL 
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ANISOU 1612 CA THR
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THR 234 21.346 10.621 38.006 1.000 17.09
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                 ANISOU 1613 C
                                                                                                                  THR 234 1717 1865 2912 146 211 - THR 234 22.558 10.644 38.139 1.000 17.25
                                                                                                                                                                                                                                                                                                                                                                          211 - 51
                 ATOM
                                                              1614 0
               ANISOU 1614 O THR 234 1776 1951 2828 108 200 2

ATOM 1615 CB THR 234 21.030 12.681 39.373 1.000 15.29

ANISOU 1615 CB THR 234 1667 1502 2642 -46 -149 1

ATOM 1616 OG1 THR 234 20.849 11.819 40.522 1.000 15.45
                                                                                                                                                                                                                                                                                                                                                                          200 229
                                                                                                                                                                                                                                                                                                                                                                        -149 1 6 3
               ANISOU 1616 OG1 THR 234 1659 1708 2502 -80 59 4 4
                ATOM 1617 CG2 THR
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ANISOU 1617 CG2 THR 234 1564
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     ANISOU 1618 N
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                           GLY
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     ATOM
               1619 CA
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    ANISOU 1619 CA GLY
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    MOTA
               1620 C
                                                             2586 133
                           GLY
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    ATOM
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    ANISOU 1621 O
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    ATOM
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    ANISOU 1622 N
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236 22.080 7.673 41.520 1.000 17.27
                          GLY
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    ATOM
              1623 CA
    ANISOU 1623 CA GLY
    ATOM
    ANISOU 1624 C
    ATOM
   ANISOU 1625 O
   ATOM
   ANISOU 1626 N
   ATOM
   ANISOU 1627 CA GLN
   ANISOU 1628 C
   ATOM
            1629 O GLN 237 24.183 12.382 44.164 1.000 18.1/
1630 CB GLN 237 24.456 11.855 41.217 1.000 17.17
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1632 CD GLN 237 1680 2833 2979 104 317 3 0
   ANISOU 1629 O
  ATOM
  ANISOU 1630 CB GLN
  ANISOU 1631 CG GLN
  ATOM
  ANISOU 1632 CD GLN
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237 24.986 12.399 38.027 1.000 18.53
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  ANISOU 1633 OE1 GLN
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            1634 NE2 GLN
  ANISOU 1634 NE2 GLN
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238 22.221 11.359 43.807 1.000 14.75
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  ANISOU 1635 N
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                        VAL
  ATOM
            1636 CA VAL
 ANISOU 1636 CA VAL
 ATOM
           1637 C
                        VAL
 ANISOU 1637 C
                        VAL
                               238 1414
 ATOM
           1638 O
                                               1392
                                                          2346 82 55 - 149
 ANISOU 1638 O VAL 238 1655 1639 2737 -218 -285 -2

ATOM 1639 CB VAL 238 20.467 13.061 44.309 1.000 14.73

ATOM 1640 CG1 VAL 238 1817 1626 2152 35 -437 -95
                               238 20.136 10.174 45.302 1.000 15.87
                       VAL
                                                                    -218 -285 - 22
                                                         2152 35 -437 - 95
 ANISOU 1640 CG1 VAL 238 1965 1490
          1641 CG2 VAL 238 21.064 13.994 43.280 1.000 16.82
ANISOU 1641 CG2 VAL 238 1862 1718 2812 -60 -378 2
ATOM 1642 N LYS 239 21.119 11.153 47.071 1.000 14.47
                                                                          -524 - 423
                                                                          -378 2 2 2
                             239 1704 1474 2318 14 -40 1 2
239 20.470 10.360 48.104 1.000 14.43
          1643 CA LYS
ANISOU 1643 CA LYS
                              239 1460 1617 2406 106 -168 1
239 19.048 10.852 48.409 1.000 14.82
ATOM
          1644 C
                       LYS
                                                                           -168 1 7 9
ANISOU 1644 C
                              LYS
ATOM
          1645 O
                       LYS
                                                                           -53 232
ANISOU 1645 O
                       LYS
                              239 1841
ATOM
          1646 CB
                              239 1841 1442 2318 158 -275 1
239 21.320 10.435 49.385 1.000 16.40
ANISOU 1646 CB LYS
                      LYS
                                                                          -275 1 9 0
                     LYS 239 1995 1712 2527 243
LYS 239 20.767 9.549 50.498 1.00
LYS 239 1954 1759 2614 -58
ATOM 1647 CG
ANISOU 1647 CG
                                                                         -543 2 5 2
                                                         50.498 1.000 16.65
                                                                         -781 2 4 4
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						- 67 -			
MOTA	1648	CD	LYS	239	21.738	9.511	51.683	1.000	19.76
ANISOU			LYS	239	2954	1820	2732	-123	-1234 3 6 3
ATOM	1649		LYS	239	21.107	8.835	52.896		
ANISOU			LYS	239	3331	2164	3086	-652	-1502 863
ATOM	1650		LYS	239	21.904	8.883	54.145	1.000	23.13
ANISOU			LYS	239	2817	3360	2612	-471	-943 2 8 7
ATOM	1651		ALA	240	18.140	9.892	48.659		14.35
ANISOU ATOM	1651 1652		ALA	240	1429	1607	2418	-156	-334 - 61
ANISOU			ALA ALA	240 240	16.791 1463	10.192 1635	49.145		13.98
ATOM	1653		ALA	240	16.728	9.776	2210	-151	-335 - 10
ANISOU			ALA	240	1439	1388	50.605 2279	$\frac{1.000}{77} - 49$	13.44
ATOM	1654		ALA	240	16.514	8.592	50.913		50 2 2 16.32
ANISOU	1654	0	ALA	240	1932	1567	2699	-215	-673 3 1 4
ATOM	1655		ALA		15.712	9.565	48.268	1.000	15.21
ANISOU	1655		ALA	240	1510	1962	2306	-104	-387 - 307
ATOM	1656		PRO	241	16.907	10.701	51.546		14.23
ANISOU			PRO		1634	1551	2221	-87	-292 7 1
ATOM	1657		PRO		17.035	10.251	52.940		14.68
ANISOU ATOM	1657		PRO	241	1718	1681	2180	-350	-174 - 30
ANISOU	1658		PRO PRO		15.693	9.961			13.89
ATOM	1659		PRO		1659 14.629	1581 10.527	2039	-107	
ANISOU			PRO	241		1946	2838	17 -29	17.06
ATOM	1660		PRO		17.689	11.462			54 146 16.63
ANISOU	1660		PRO		2162	1657	2501	-460°	-487 5 5
ATOM	1661		PRO	241	17.138	12.651	52.826		16.56
ANISOU			PRO		-2433	1601	2258	-367	-274 3 1
ATOM	1662		PRO		17.164	12.140			14.92
ANISOU ATOM	1662 1663		PRO		1841	1490	2339	-215	-186 - 66
ANISOU			ARG ARG		15.740	9.049			15.74
ATOM	1664		ARG		1914 14.574	1853 8.772	2212	-381	-308 2 0 4
ANISOU	1664		ARG	242	1955	1863	55.376 2073	-236	15.50 -291 1 8 0
ATOM	1665		ARG	242	14.406	9.841			16.60
ANISOU			ARG		1889	2011	2407	-120	-411 - 51
ATOM	1666		ARG		15.372	10.416	56.994		18.31
ANISOU			ARG	242	2041	2186	2732	-216	-559 - 180
ATOM	1667		ARG	242	14.728	7.419	56.085		18.38
ANISOU	1667		ARG		2920	1810	2253	-486	-391 2 6 9
ATOM ANISOU	1668		ARG		14.564	6.273			18.42
ATOM	1669		ARG ARG		2372 14.854	1873	2755		162 - 155
ANISOU			ARG		3380	4.935 2022	3366	470	23.07
ATOM	1670		ARG		16.334	4.954			-483 - 217 26.69
ANISOU			ARG		3498	2727	3916	444	-829 4 7
ATOM	1671		ARG		16.941	3.921			27.19
ANISOU			ARG	242	3166	2879	4284	-297	-1143 802
ATOM	1672	NH1	ARG		16.157	2.913			33.14
ANISOU	1672	NH1	ARG	242	3810	3235	5546	-316	528 726
ATOM	1673	NH2	ARG	242	18.241	3.889			31.13
ANISOU ATOM	1674				3043	2925	5859	227	-769 4 8 4
ANISOU			HIS HIS	243	13.188 1979	10.057	56.872		17.55
ATOM	1675		HIS		12.913	2233 11.050	2457 57 914	-165 1 000	-173 - 74 17.84
ANISOU	1675	CA	HIS	243		2139	2452	-260	-123 - 75
ATOM	1676	С	HIS	243	11.644	10.627	58.643		17.52
ANISOU			HIS	243	2102	2084	2470	-248	-164 - 325
ATOM	1677		HIS	243	10.870	9.803	58.132		20.23
ANISOU			HIS		2226	2593	2868	-551	-323 - 392
ATOM	1678	CB	HIS	243	12.865	12.456	57.324	1.000	19.74

- 68 -ANISOU 1678 CB HIS 243 2770 2248 2482 -188 -106 8 3 1679 CG HIS 243 11.922 12.630 56.187 1.000 22.60 ANISOU 1679 CG HIS 243 3449 2513 2624 164 1680 ND1 HIS ATOM 243 12.209 12.299 54.879 1.000 25.87 ANISOU 1680 ND1 HIS 243 4780 2575 2473 -609 -403 5 3 1681 CD2 HIS 243 10.633 13.034 56.172 1.000 29.11 ANISOU 1681 CD2 HIS 243 3220 4490 3348 121 -421 1630 1682 CE1 HIS 243 11.182 12.573 54.109 1.000 32.92 ANISOU 1682 CE1 HIS 243 5835 3672 3001 -1102 -1367 689 1683 NE2 HIS 243 10.214 13.012 54.875 1.000 36.95 ANISOU 1683 NE2 HIS ATOM 1684 N HIS 244 2523 2477 2171 -88 -141 -117 244 10.302 10.801 60.649 1.000 20.83 ANISOU 1684 N HIS MOTA 1685 CA HIS ANISOU 1685 CA HIS 244 2802 2485 2628 171 251 2 7 2 244 9.927 11.968 61.551 1.000 20.33 244 1803 2969 2953 -31 -78 - 2 7 ATOM 1586 C HIS 244 1803 2969 2953 -31 -78 -2 244 10.482 13.073 61.510 1.000 21.71 244 2057 3418 2774 ANISOU 1686 C HIS -78 - 2731687 O HIS ANISOU 1687 O HIS 244 2057 3418 2774 -535 145 -8 244 10.714 9.557 61.468 1.000 24.38 244 4066 2644 2553 -76 -390 4 145 - 853 1688 CB HIS ATOM ANISOU 1688 CB HIS 244 4066 2644 2553 -76 -390 4 244 11.859 9.725 62.423 1.000 28.34 244 4158 3498 3113 696 -727 -244 13.132 9.205 62.268 1.000 32.35 244 4012 4471 3808 548 -485 -8 -76 -390 4 4 1 ATOM 1689 CG HIS ANISOU 1689 CG HIS **-**727 **-** 8 9 1690 ND1 HIS ANISOU 1690 ND1 HIS 244 4012 4471 3808 548 -485 -850 ATOM 1691 CD2 HIS 244 11.928 10.391 63.609 1.000 25.21 240 11.000 1691 CD2 HIS 244 2937 4137 2505 -373 45 21 9 ATOM 1692 CE1 HIS 244 413.887 4277 3613 1224 -749 -51 8 ATOM 1693 NE2 HIS 244 4157 4277 3613 1224 -749 -51 8 ATOM 1693 NE2 HIS 244 13.146 10.263 64.150 1.000 24.52 ATOM 1694 N VAL 245 8.890 11.687 62.349 1.000 23.87 ATOM 1695 CA VAL 245 8.890 11.687 62.349 1.000 23.87 ATOM 1696 C VAL 245 8.473 12.691 63.349 1.000 24.85 ATOM 1696 C VAL 245 8.624 12.079 64.735 1.000 24.85 ATOM 1696 C VAL 245 8.624 12.079 64.735 1.000 26.03 ATOM 1697 O VAL 245 8.023 11.025 84.896 11.025 84.896 1.000 27.98 ATOM 1698 CB VAL 245 3120 3085 4428 42 295 -59 ATOM 1699 CG1 VAL 245 8.023 11.025 64.969 1.000 27.98 ATOM 1699 CG1 VAL 245 2621 3489 3777 94 -103 -569 ATOM 1699 CG1 VAL 245 2621 3489 3777 94 -103 -569 ATOM 1699 CG1 VAL 245 2621 3489 3777 94 -103 -569 ATOM 1699 CG1 VAL 245 2621 3489 3777 94 -103 -569 ATOM 1699 CG1 VAL 245 2621 3489 3777 94 -103 -569 ATOM 1700 CG2 VAL 245 3564 3809 4220 1264 -305 - 33 ATOM 1700 CG2 VAL 245 3564 3809 4220 1264 -305 - 33 ATOM 1701 N ALA 246 9.399 12.696 65.603 1.000 27.45 ATOM 1701 N ALA 246 9.399 12.696 65.603 1.000 27.45 ATOM 1702 CA ALA 246 9.399 12.696 65.603 1.000 27.45 ATOM 1703 C ALA 246 4363 3360 2707 292 275 373 73 ATOM 1703 C ALA 246 4363 3360 2707 292 275 373 373 ATOM 1704 O ALA 246 4363 3360 2707 292 275 373 373 ATOM 1704 O ALA 246 4363 3360 2707 292 275 373 373 ATOM 1704 O ALA 246 4363 3360 2707 292 275 373 373 ATOM 1704 O ALA 246 4363 3360 2707 292 275 373 373 ATOM 1704 O ALA 246 4363 3360 2707 292 275 373 373 ATOM 1704 O ALA 246 47.774 313.791 67.563 1.000 29.54 428 370 3031 98 880 197 7 224 875 -329 420 1704 O ALA 246 47.774 313.791 67.563 1.000 29.54 428 370 3031 98 880 197 7 224 875 -329 420 1704 O ALA 246 47.774 313.791 67.563 1.000 29.54 428 370 3031 38 370 3000 27.45 5 370 3000 27.45 5 370 3000 27.45 5 370 3000 27.45 5 370 3000 27.45 5 370 3000 27.45 5 370 3000 27.45 5 370 3000 27.45 5 370 3000 27.45 5 370 3000 27.45 5 ANISOU 1690 ND1 HIS -485 - 8501691 CD2 HIS 3417 -224 875 -329 1705 CB ALA 246 10.819 13.010 67.542 1.000 30.33 ANISOU 1705 CB ALA 246 4564 3949 3011 615 -221 - 422 1706 N ALA 247 8.048 11.958 ANISOU 1706 N ALA 247 4483 68.849 1.000 34.09 5156 3311 -1190 466 3 9 3 1707 CA ALA 247 7.036 12.190 69.859 1.000 34.23 ANISOU 1707 CA ALA 247 4188 5627 3189 -1215 315 515 12.910 71.081 1.000 33.31 4684 2555 249 -506 1 ATOM 1708 C ANISOU 1708 C ALA247 7.609 ALA247 5419 -506 1 1 4 7

ATOM ANISOU	1710 CB 1710 CB 17110 CB 17111 N CA 17112 CC 17113 CO 17114 CCA 17115 CC 17115 CC 17116 CCC 17117 CC 17117 CC 17118 N CC 17119 CC 17	ARG ARG ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	247 78 78 78 78 78 78 78 78 78 78 78 78 78	-69 - 12.78 1 167.28 1 167.28 1 167.28 1 154.58 1 154.58 1 154.58 1 154.58 1 154.58 1 154.58 1 154.60 9 1 155.64 1 155.64 1 155.64 1 155.64 1 155.64 1 155.64 1 155.64 1 155.64 1 155.64 1 155.64 1 155.68 1 171.27 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	4259 70.31 71.36 72.37 73.36 73.37 73.37 73.37 73.37 73.37 73.37 73.37 73.37 73.37 74.37 74.37 75.52 75.45 71.06 71.06 73.56 73.37 74.37 75.57 77.12 77.12 77.13 77.	-378 1.000 -3000 1.000 -1.	45.48 2573 - 796 49.75 1238 - 138 50.89 2210 - 1064 44.69 953 - 577 48.76 1069 - 477 55.51 895 566 46.09 -7 1237 56.25 1799 3 9 9 5 55.24 2864 1270 71.04 3707 6 2 2 72.89 2723 4 0 9 70.73 2650 - 266 72.71 2153 1 3 3 89.50 1622 3 8 7 4 67.68 3886 2 2 1 85.24 -1437 2 3 4 7 76.08 1617 15 9 2 60.91 2886 1 3 1 2 72.37 4553 3 3 8 1 60.48 4570 - 1 1 1 2 54.40 2922 - 9 4 0 40.05 836 - 9 2 1 38.82
ATOM ANISOU ATOM ANISOU ATOM	1734 N 1735 CA 1735 CA 1736 C 1736 C 1737 O	GLY GLY GLY GLY GLY	255 8029 255 2.880 255 5181 255 3.640 255 4227 255 4.580	5451 23.171 4570 22.565 4772 23.163	7190 74.098 5465 72.921 5749 72.398	594 1.000 1424 1.000 557	2922 - 940 40.05 836 - 921
ATOM	1737 O 1738 N 1738 N 1739 CA	GLY SER SER SER	255 2978 256 3.164 256 5047 256 3.738	6491 21.387 4594 20.606	5715 72.509 4527	-128 1.000 389	-136 -2226 37.29

- 70 -

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ANISOU 1739 CA SER
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ANISOU 1740 C
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ANISOU 1742 CB
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                         SER
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ANISOU 1743 OG SER
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ANISOU 1744 N
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ATOM
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                                                                68.767 1.000 30.95
ANISOU 1745 CA SER
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                                                   5827
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                                                                                      672 - 509
            1746 C
MOTA
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                                                     22.538 67.760 1.000 30.63
ANISOU 1746 C
                                  257 3181 5524
                          SER
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257 3500 6070
            1747 O
ATOM
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ANISOU 1747 O
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257 3085 6518 5103 796 1381 4
ATOM
            1748 CB
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ANISOU 1748 CB
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ATOM 1749 OG SER 257 0.801 24.361 68.601 1.000 65.12 ANISOU 1749 OG SER 257 8002 5175 11565 -999 -3375 ATOM 1750 N ARG 258 2.119 22.384 66.471 1.000 30.51 ANISOU 1750 N ARG 258 3668 5068 2855 -332 677 - ATOM 1751 CA ARG 258 2.997 22.819 65.396 1.000 28.15 ANISOU 1751 CA ARG 258 3100 4620 2976 -106 358 - ATOM 1752 C ARG 258 2.198 22.913 64.096 1.000 25.64 ANISOU 1752 C ARG 258 3488 3381 2872 -676 273
                                                                                      1381 4 3 5
                                                                                     -3375 383
                                                                            -332 677 -995
                                                                            -106 358 -544
ANISOU 1752 C
                                  258.3488 3381 2872 -676 273 -
258.1.132 22.294 63.981 1.000 24.93
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ATOM
           1753 0

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      63.981
      1.000
      24.93

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      27.21

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ANISOU 1753 O
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ATOM
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ANISOU 1754 CB
                         ARG
           1755 CG
MOTA
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ANISOU 1755 CG
                         ARG
            1756 CD
MOTA
                         ARG
ANISOU 1756 CD
                         ARG
ATOM
            1757 NE
                         ARG
ANISOU 1757 NE
                         ARG
           1758 CZ
ATOM
                         ARG
ANISOU 1758 CZ
                         ARG
ATOM
           1759 NH1 ARG
ANISOU 1759 NH1 ARG
           1760 NH2 ARG
ATOM
ANISOU 1760 NH2 ARG
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ANISOU 1761 N
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ATOM
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ANISOU 1762 CA
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ANISOU 1763 C
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MOTA
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ANISOU 1764 O
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ATOM
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ANISOU 1765 CB
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ANISOU 1766 OG1 THR
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MOTA
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ANISOU 1767 CG2 THR
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                                                                            726
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MOTA
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ANISOU 1768 N
                          SER
                                  260 2386
                                                     2762
                                                                  2609
                                                                             -61
                                                                                      74 - 806
           1769 CA
MOTA
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ANISOU 1769 CA
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                                  260 2488
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22.750
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ANISOU 1772 CB
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ATOM
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ATOM
ANISOU 1785 CG1 VAL
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ANISOU 1786 CG2 VAL
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ANISOU 1796 CE2 PHE
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ANISOU 1797 CZ
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ANISOU 1799 CA PHE
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     1800 C
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						- 72 -		
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ANISOU			PHE		1165	1473	2133	-77 -120 4 6
ATOM	1802		PHE		5.346	17.099	46.773	1.000 12.39
ANISOU			PHE		1101	1498	2110	-304 -42 6 3
ATOM	1803		PHE		5.022	16.558		1.000 13.97
ANISOU			PHE		1647	1465	2197	-290 13 1 2 1
ATOM ANISOU	1804				5.960	15.848		1.000 17.07
ANISOU	1804				2039	1976		-422 -410 4 9 7
ANISOU					3.747 1835	16.679		1.000 17.41
ATOM	1806				5.661	2359 15.247	2419	-440 433 112
ANISOU					2616	2710	2496	1.000 20.59
ATOM	1807				3.458	16.133		-556 -425 7 2 5 1.000 22.51
ANISOU					2151	4047	2355	-787 106 553
ATOM	1808		PHE	264	4.386	15.350		1.000 20.88
ANISOU	1808	CZ	PHE		2889	2376	2669	-936 -22 3.06
ATOM	1809		LEU	265	7.676	18.756		1.000 11.81
ANISOU			LEU		1192	1248	2047	-37 47 1 9
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ANISOU			LEU		1264	1269	2028	-223 16 -63
ATOM	1811		LEU	265	7.915	17.617	42.703	1.000 12.10
ANISOU ATOM			LEU	265	1266 .	1298		-117 -81 3
ANISOU	1812		LEU LEU	265	8.842	16.834		1.000 12.93
ATOM	1813		LEU		1367 9.246	1283	2260	-107 -152 4 4
ANISOU			LEU		1399	19.730 1364		1.000 12.59
ATOM	1814		LEU		9.500	20.124	2019	-257 57 - 9 1.000 12.19
ANISOU			LEU		1168	1399		-292 -248 3 0 2
ATOM	1815			265	8.620	21.314		1.000 13.29
ANISOU	1815	CD1	LEU		1518	1546	1984	84 36 1 9
MOTA	1816	CD2	LEU		10.971	20.458		1.000 13.14
ANISOU			LEU	265	1204	1593	2197	-234 41 - 20
ATOM	1817		ARG		6.842	17.249		1.000 12.06
ANISOU			ARG		1412	1127		-220 -190 4 5
ATOM	1818		ARG		6.586	15.913		1.000 12.07
ANISOU ATOM			ARG		1372	1201	2012	-258 0 8 0
ANISOU	1819		ARG		6.619	15.965	39.972	1.000 11.75
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ANISOU			ARG		1142	1477	2302	-189 43 - 33
ATOM	1822		ARG		5.036	15.606	43.488	1.000 13.80
ANISOU	1822	CG	ARG		1351	1686	2207	-159 66 -115
ATOM	1823		ARG		3.723	15.041		1.000 12.70
ANISOU			ARG		1369	1362	2094	66 -22 8 4
ATOM	1824		ARG		2.581	15.648	43.281	1.000 12.97
ANISOU			ARG		1343	1155	2428	52 -165 -137
ATOM	1825	CZ	ARG		1.304	15.281		1.000 11.34
ANISOU ATOM			ARG		1432	1009	1869	45 -149 -103
	1826 1826			266	0.995	14.414		1.000 13.39
ATOM	1827	MHO	ARG	266	1802	1165	2119	-11 -38 7 2
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ATOM	1829		PRO	267		14.947		1.000 13.88
ANISOU			PRO	267		1786	2047	167 -125 - 84
ATOM	1830	С	PRO		5.957	14.722		1.000 12.61
ANISOU	1830	С	PRO	267	1413	1508	1868	-6 44 2 7
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ATOM 1852 CB ANISOU 1852 CB ATOM 1853 CG ANISOU 1853 CG ATOM 1854 ODD ANISOU 1855 ODD ATOM 1855 ODD ATOM 1856 N ANISOU 1856 N ANISOU 1857 CA ANISOU 1858 C	ASN 268 2573 268 6.066 2 ASN 268 2408 ALA 269 3.531 ALA 269 1677 ALA 269 1459 ALA 269 4.189 ALA 269 4.581 ALA 269 1718 ALA 269 1300 ASP 270 4.488 ALA 269 1300 ASP 270 5.247 ASP 270 5.247 ASP 270 1747 ASP 270 6.749 ASP 270 7.488 ASP 270 1714 ASP 270 4.618 ASP 270 4.646 ASP 270 3317 ASP 270 3424 ASP 270 3424 ASP 270 3317 ASP 270 4.646 ASP 270 3317 ASP 271 1556 ASP 271 1624 ASP 271 1624 ASP 271 9.27	1355 2164 13.761 37.599 1740 2637 12.846 38.764 1804 2324 13.746 39.965 1356 2438 15.051 35.939 1665 1777 14.709 35.073 1401 2018 13.192 34.873 1350 2156 12.467 34.934 1416 2167 15.338 33.69 1369 2162 17.454 34.352 1467 2172 1439 2162 17.454 34.352 1467 2172 1467 234.594 11.286 34.353 1476 2494 11.051 34.008 1478 2454 11.079 31.098 11.086 2288 13.168 29.809 1476 2300 1476 2300 1476 230.649 1541<	1.000 15.41 -17 -184 4 7 1.000 17.75 42 91 - 9 8 1.000 16.61 -50 -57 1 4 2 1.000 13.99 -356 -65 1 7 0 1.000 13.42 -208 -118 1 0 7 1.000 13.93 -168 -5 1 5 3 1.000 14.97 -143 112 8 6 1.000 13.76 -60 -61 1 2 3 1.000 14.38 -151 30 - 5 1.000 14.83 -99 -42 6 8 1.000 15.68 -224 143 8 6 1.000 17.12 -80 139 2 2 6 1.000 17.67 -75 -319 1 2 6 1.000 17.67 -75 -319 1 2 6 1.000 18.22 -88 -80 4 7 4 1.000 20.55 -47 -287 4 2 5 1.000 23.06 -49 -136 8 1 2 1.000 13.93 97 31 4 1 110 29 2 6 3 1.000 13.31
ATOM 1856 N ANISOU 1856 N ATOM 1857 CA ANISOU 1857 CA	PHE 271 7.223 PHE 271 1556 PHE 271 8.673 PHE 271 1624	11.668 32.413 1318 2417 11.723 32.644 1430 2423 10.349 32.325 1430 2225 9.340 32.870 1374 2392 12.146 34.098 1721 2495	97 31 4 1 1.000 14.41 110 29 263

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- 74 -
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          1876 C
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                    PHE

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ANISOU 1890 OG
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ANISOU 1891 N
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ATOM	1893 C	VAL	275 16.454	0.445		1.000 15.33
ANISOU	1893 C	VAL	275 1805	1881	2139	116 392 - 45
ATOM	1894 0	VAL	275 16.623	0.280	34 971	1.000 15.68
ANISOU	1894 0	VAL	275 2037	1655		
ATOM	1895 CB	VAL	275 14.227	-0.004	220/	6 297 1 9 6
ANISOU		VAL	275 1635	1708	2755	1.000 16.05
ATOM	1896 CG:	L VAL	275 14.080	-1.186		-76 4 05 2 1
	1896 CG	VAT.	275 2045	1688	2740	1.000 17.04
ATOM	1897 CG:	VAI.	275 12.847	0.608		-211 230 1 5
ANISOU		VAI.	275 1650	2432	2928	1.000 18.45
ATOM	1898 N	PRO	276 17.437	0.093		-57 135 269
ANISOU	1898 N	PRO	276 1927	1700	2532	1.000 16.21
ATOM	1899 CA	PRO	276 18.707	-0.434		97 589 3 6
ANISOU		PRO	276 1736	2115	3025	1.000 18.10
ATOM:	1900 C	PRO	276 19.382	0.541		147 616 - 93 1.000 17.52
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ATOM	1901 0	PRO	276 19.963	0.171		97 469 2 3 9 1.000 19.66
ANISOU	1901 0	PRO	276 2015	2409	3047	24 280 4 6 8
ATOM	1902 CB	PRO	276 19.590		3047	1.000 20 . 80
ANISOU	1902 CB	PRO	276 2094	2687	3121	
ATOM	1903 CG	PRO	276 18.852	-0.390	30 999	306 771 - 249 1.000 21.57
ANISOU	1903 CG	PRO	276 2051	3098	3046	
MOTA	1904 CD	PRO	276 17.446	-0.021	31 368	340 802 - 288 1.000 18.17
ANISOU	1904 CD	PRO	276 2053	2306	2546	179 832 -318
ATOM	1905 N	LEU	277 19.325	1.845	34 027	1.000 17.09
ANISOU	1905 N	LEU	277 1571	1898	3025	230 511 107
ATOM	1906 CA	LEU	277 19.962	2.802	34.940	1.000 19.34
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ATOM	1910 CG	LEU	277 20.910			1.000 26.34
	1910 CG	LEU	277 3662	5.192 2367	3978	-980 -547 9 4 4
ATOM	1911 CD1	LEU	277 22.396	4.839	35.069	1.000 38.04
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ATOM	1912 CD2	LEU	277 20.708	6.607	34.631	1.000 31.98
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	1913 N	ALA	278 2015	1766	2793	74 218 1 1 5
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	1915 C 1915 C	ALA	278 17.575	1.523	38.313	1.000 16.31
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	1916 0	ALA	278 17.718	1.635	39.523	1.000 17.26
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	1917 CB	ALA	278 15.642	2.622		1.000 17.55
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ATOM	1921 O 1922 CB	ARG	279 3615	4823	4115	-1726 -1700 2603
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ANISOU ATOM OU ANISOU A	1922222222222233445566778889900112233344556677888990001 1992222222222223334455667788899001 1199999999999933333333333333333333	GGDDEEN HILLSONNUNN OCCOOOCCOOCCOONNOCCOOOCCSSNNCCCOOONNOCCOOONNOCCOOOCCSSNNCCCOOONNOCCOO	ARGUUUUUUUUUUUUUUUUUUUUUUUUUUUUUUUUUUUU	277999999000000000000000000000000000000	9516 20.390 2172 21.748 2046 21.705 2334 22.723 2659 22.651 2778 22.997 2605 24.541 2666 23.727 10844 20.777 20.481 2114 19.858 24.92 19.789 19.789 19.632 19.789 19.632 10822 19.789 19.632 10822 10823 10823 10823 10823 10823 10823 10824 10825 10825 10826 10826 10826 10827 10826 10827 10827 10828 10848	-76- 160.491 2728-294.484 265.762-3.42-4.46 265.766.01 276.01.68 20.119 20.334 1.2534 1.268 1.278 1.278 1.278 1.278 1.278 1.278 1.278 1.278 1.288 1.288 1.288 1.288 1.288 1.288 1.288 1.288 1.288 1.288 1.288 1.288 1.38	2353366667488295829799999506677466673266665188.33333333333333333333333333333333333	1.000 -98 1.000	20.73 -401-351 24.81 507-609 27.50 -146-181 41.33 -454-142 40.58 507 4 5 2 53.27 -4607-463 19.68 4136 20.28 1115 20.67 285 2 0 26.81 -183-87 24.69 1022 3 0 3 27.13 116 6 2 3 43.10 1206 8 3 4 41.36 99 6 9 0 64.81 1104 2 1 3 4 21.61 532-2 3 8 24.33 1121-817 27.11 1457-1343 19.19 -326 1 3 5 22.02 100-2108 53.41 1316 4 5 18.81 49-206 17.07 52-168 14.91 -453 3 7 8 16.38 -399 3 6 0 13.44 -336-115 14.52 -670 4 6 13.08 -338 1 7 4	
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ATOM 2003 O GLU 290 2180 2308 2313 50 711 -297

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ANISOU 2013 CB THR 291 3043 2625 2516 -164 891 362
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ATOM	2018		ALA		9.356	5.065		
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ATOM	2019						1908	60 144 - 139
			ALA		10.228	5.939		1.000 14.27
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ANISOU	2021	N	THR	293	1468	1617	2058	117 373 -118
ATOM	2022	CA	THR		7.605	6.546		1.000 13.40
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ATOM	2023		THR				1877	152 209 -232
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ANISOU	2026	OG1	THE	293	1672	1570	1981	
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\mathtt{ATOM}	2029		PHE	294	6.857	7.773	35.935	1.000 12.37
ANISOU	2029	CA	PHE	294	1332	1469	1899	-267 166 -289
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ANISOU			PHE		1336	1361	1999	-151 30 - 36
ATOM	2031		PHE		5.403	6.253		
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ATOM	2033		PHE		6.306	9.488	37.711	1.000 13.10
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MOTA	2034			294	7.207	9.411	38.749	1.000 17.41
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ANISOU	2035	CD2	PHF		2156	2263	2575	
ATOM	2036			204	6.810			
ANISOU	2030	CEI	DUD			9.608		1.000 17.72
	2030	CEI	PRE		2348	2296	2086	-308 -362 -136
ATOM		CEZ	PHE		4.591	10.010	39.324	1.000 19.37
ANISOU	2037	CE2			2078	2541	2740	330 232 -630
MOTA	2038		PHE	294	5.507	9.956	40.355	1.000 18.36
ANISOU	2038	CZ	PHE	294	2443	1678	2855	-394 -55 -245
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ATOM	2044		GLN		1.062	6.256		1.000 14.03

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ANISOU					1757	1937	2106	-229 137 177
ATOM	2056		TRP		6.038	3.352	36.416	1.000 12.26
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ANISOU	2060	СВ	TRP	297	1130	1692	2376	-19 -169 1 5 1
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ATOM	2063	CD2	TRP		9.144	4.353	40 100	1.000 14.69
ANISOU	2063	CD2	ጥጽ₽		1327	1693	2562	
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ATOM	2067	C72	ם מעד		10.318	1008	3712	
ANISOU	2067	C72	WD D		10.318			1.000 18.45
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ATOM	2071		ILE		4.299	4.440		1.000 14.68
ANISOU			ILE		1413	2177	1986	-13 -161 -208
ATOM	2072	C	ILE		2.841	4.054	40.121	1.000 12.02
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ATOM 2075 CG1 ILE 298 5.907
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ATOM 2076 CG2 ILE 298 3.679
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ANTSOU 2079 CA GLY 299 1.756 1279 2379 106 -188 -154  
ATOM 2080 C GLY 299 1.135 5.017 38.378 1.000 13.09  
ANTSOU 2081 O GLY 299 0.738 6.025 38.017 1.000 14.00  
ANTSOU 2081 O GLY 299 1.713 1353 2252 122 289 -13  
ANTSOU 2082 N GLY 300 -1.183 4.917 38.447 1.000 13.08  
ANTSOU 2082 N GLY 300 1325 5.966 37.992 1.000 13.45  
ANTSOU 2083 CA GLY 300 1.255 5.966 37.992 1.000 13.45  
ANTSOU 2083 CA GLY 300 1.251 6.972 39.042 1.000 12.94  
ANTSOU 2084 C GLY 300 1.998 7.875 38.672 1.000 13.45  
ANTSOU 2085 O GLY 300 1.321 1342 2423 -19 -217 -45  
ANTSOU 2086 N ASN 301 -3.052 7.842 41.313 1.000 13.39  
ANTSOU 2086 N ASN 301 1.590 1435 2230 -194 -38 -61  
ANTSOU 2088 C ASN 301 1.676 1268 1791 -35 -144 -13  
ANTSOU 2088 C ASN 301 1.676 1268 1791 -35 -144 -13  
ANTSOU 2089 O ASN 301 1.676 1268 1791 -35 -144 -13  
ANTSOU 2089 O ASN 301 1.632 1909 2542 77 224 3 15  
ANTSOU 2090 CB ASN 301 1.301 -3.098  
ANTSOU 2090 CB ASN 301 1.306 1.307  
ANTSOU 2090 CB ASN 301 1.308 1.355 2093 73 -144 -13  
ANTSOU 2091 CG ASN 301 1.308 1.355 2093 73 -144 -13  
ANTSOU 2091 CG ASN 301 1.309 1.309  
ANTSOU 2099 C TYR 302 1.662 1278  
ANTSOU 2099 C TYR 302 1.676 1268 1279  
ANTSOU 2099 C TYR 302 1.676 1228 1229  
ANTSOU 2099 C TYR 302 1.635 1229  
ANTSOU 2099 C TYR 302 1.586 1229  
ANTSOU 2090 C TYR 30
    MOTA
    ANISOU 2079 CA GLY
    MOTA
                                      2080 C
                                                                                    GLY
                                                                                                               302 1581 1043 2045 -185 -84 - 77
302 0.637 13.273 39.535 1.000 14.12
302 1462 1443 2458 -241 15 3 2 5
302 1.983 13.347 39.241 1.000 12.69 3
302 1483 1224 2113 -287 -91 1 0
      ANISOU 2102 CE1 TYR
     ATOM 2103 CE2 TYR
ANISOU 2103 CE2 TYR
                                           2104 CZ TYR
      ANISOU 2104 CZ TYR
                                                                                                                302 2.376 13.866 38.013 1.000 13.42
      ATOM 2105 OH TYR
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- 82 -302 1505 303 1.956 ANISOU 2105 OH TYR 1469 2124 -93 33 1 4 6 44.450 1.000 13.92 2106 N VAL 8.855 MOTA ANISOU 2106 N VAL 303 1406 1637 2246 153 88 9 9 45.746 1.000 14.51 MOTA 2107 CA VAL 303 2.355 8.336 303 1838 303 3.498 303 1404 ANISOU 2107 CA VAL 1320 -137 -391 - 74 2355 9.244 2108 C VAL 46.239 1.000 15.23 ANISOU 2108 C VAL 1507 2876 -102 -105 -348 2109 O 303 4.471 9.386 MOTA VAL 45.512 1.000 18.70 ANISOU 2109 O 303 1859 VAL 1861 3386 -239 326 -504 303 2.856 303 2140 303 3.279 ATOM 2110 CB VAL ANISOU 2110 CB VAL 6.880 45.632 1.000 16.75 1319 2905 16 -759 -123 6.401 47.017 1.000 19.53 2111 CG1 VAL MOTA ANISOU 2111 CG1 VAL 303 2185 1951 3284 232 -1054 1 4 8 MOTA 2112 CG2 VAL 303 1.723 5.956 45.125 1.000 17.82 ANISOU 2112 CG2 VAL 303 2476 304 3.349 1442 2852 -213 -558 - 406 MOTA 2113 N ASN 47.378 1.000 14.07 ANISOU 2113 N 304 1409 1369 ASN 2566 -39 -407 - 86 2114 CA ASN 304 4.317 10.928 47.772 1.000 14.31 304 1474 ANISOU 2114 CA ASN 1387 2578 -102 -424 - 5 5 10.397 48.637 1.000 13.75 ATOM 2115 C ANISOU 2115 C 304 5.450 304 1360 ASN 1487 2378 34 -274 - 87 10.962 48.584 1.000 14.60 ASN ATOM 2116 0 ASN 304 6.539 ANISOU 2116 O ASN 304 1314 1795 2438 -34 -55 -320 304 3.589 304 1710 304 2.535 MOTA 2117 CB ASN ANISOU 2117 CB 2494 6 -303 176 1214 ASN 1214 2494 6 -303 176 12.661 47.642 1.000 14.81 2118 CG ASN ATOM 304 1551 ANISOU 2118 CG ASN 1627 2449 23 -114 402 13.255 46.622 1.000 16.52 2119 OD1 ASN 304 2.866 ANISOU 2119 OD1 ASN 304 1896 304 1.290 304 1560 2120 ND2 ASN ANISOU 2120 ND2 ASN 9.413 2121 N 305 5.175 ATOM ILE ANISOU 2121 N ILE 305 1546 1553 3117 -78 -503 2 6 6 305 6.173 305 1670 ATOM 2122 CA ILE ANISOU 2122 CA ILE 8.890 50.407 1.000 14.85 1537 7.372 2436 165 -277 - 4 0 50.352 1.000 15.78 305 6.183 2123 C ATOM: ILE 305 1527 2914 95 -438 - 51 ANISOU 2123 C ILE 1555 49.886 1.000 17.54 2124 0 305 5.231 6.736 MOTA ILE 3412 -131 -404 5 51.818 1.000 17.80 2634 -23 265 -209 52.416 1.000 18.93 305 1463 305 5.949 305 2167 ANISOU 2124 O ILE 1789 9.430 2125 CB ILE ATOM ANISOU 2125 CB ILE 1962 2126 CG1 ILE 9.091 305 4.578 ANISOU 2126 CG1 ILE 305 1716 305 6.171 305 2685 305 4.415 MOTA 2127 CG2 ILE 10. 1863 ANISOU 2127 CG2 ILE 2128 CD1 ILE 9.459 53.863 1.000 21.28 ATOM 305 2521 306 7.246 2662 19 452 - 71 ANISOU 2128 CD1 ILE 2902 6.806 50.908 1.000 14.59 ATOM 2129 N ARG 6.00 1641 360 306 1738 306 7.424 ANISOU 2129 N ARG 2165 52 -356 271 MOTA 2130 CA ARG 50.828 1.000 15.25 1663 306 1509 1663 2622 139 -302 7 7 4.903 52.024 1.000 15.02 ANISOU 2130 CA ARG MOTA 2131 C ARG 306 8.234 1464 2656 133 -332 - 21 5.614 52.433 1.000 16.63 306 1588 306 9.141 306 1682 ANISOU 2131 C ARG MOTA 2132 0 ARG ANISOU 2132 O ARG 2133 CB 306 8.135 ATOM ARG ANISOU 2133 CB 2697 -100 -270 -150 ARG 306 1820 1681 3.414 49.377 1.000 18.43 MOTA 2134 CG ARG 306 8.226 1700 2828 40 -194 -156 3.068 47.900 1.000 18.26 1971 2880 -120 -145 -33 ANISOU 2134 CG 306 2476 ARG 1700 ARG 306 8.401 ARG 306 2087 2135 CD ANISOU 2135 CD 1971 2880 -120 -145 - 330

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- 83 -2136 NE ARG 306 7.136 MOTA 3.228 47.188 1.000 20.53 ANISOU 2136 NE ARG 306 2442 2013 3345 -577 -668 -2342137 CZ ARG 306 6.980 MOTA 3.178 45.873 1.000 20.27 ANISOU 2137 CZ ARG 306 2330 2057 3316 373 -522 2 0 2138 NH1 ARG 306 8.086 3.000 MOTA 45.107 1.000 22.13 ANISOU 2138 NH1 ARG 306 2136 2580 274 -589 - 723 3695 306 5.759 3.250 2139 NH2 ARG ATOM 45.341 1.000 18.44 ANISOU 2139 NH2 ARG 306 2107 1838 3062 259 -285 8 4 307 7.898 3.775 2140 N ATOM ARG 52.612 1.000 19.10 ANISOU 2140 N ARG 307 2716 1872 2671 -294 -607 3 2 7 MOTA 2141 CA ARG 307 8.576 3.212 53.768 1.000 21.13 ANISOU 2141 CA ARG 307 3321 2201 2504 -48 -845 1 3 9 307 9.536 2.138 53.277 1.000 23.30 2142 C ATOM ARG ANISOU 2142 C ARG 307 3417 2170 3267 181 -1046 3 9 ATOM 2143 0 307 9.385 1.601 52.187 1.000 21.01 ARG ANISOU 2143 O ARG 307 2574 2355 3052 174 -728 1 1 2 ATOM 2144 CB ARG ANISOU 2144 CB ARG 307 7.557 2.522 54.694 1.000 27.30 307 4545 3184 2645 -13 -247 7 0 5 2145 CG ATOM ARG 307 6.839 3.488 55.629 1.000 46.30 ANISOU 2145 CG 307 6310 307 7.054 307 11107 ARG 6374 4907 215 1655 - 970 2146 CD 3.085 57.085 1.000 66.50 10355 3806 -2980 2792 -3 ATOM ARG ANISOU 2146 CD ARG -2980 2792 -1145 2147 NE ATOM 307 5.989 ARG 2.203 57.531 1.000 78.91 307 11821 ANISOU 2147 NE ARG 12833 5330 -4530 1969 - 5 307 5.987 2148 CZ 1.285 ARG 58.479 1.000 73.67 ANISOU 2148 CZ ARG 307 7704 14382 5907 -4724 1249 1051 2149 NH1 ARG 307 7.063 1.038 17949 0.597 15919 59.214 1.000 80.32 ANISOU 2149 NH1 ARG 307 6613 5955 -3290 2179 1 0 5 2150 NH2 ARG 307 4.872 58.707 1.000 73.74 ANISOU 2150 NH2 ARG 307 9116 2983 -6954 438 -917 307 9116 13919 308 10.551 1.861 2151 N THR 54.113 1.000 25.61 ANISOU 2151 N THR 308 4234 2212 3285 536 -1421 - 2322152 CA THR 308 11.308 0.640 53.822 1.000 30.02 ANISOU 2152 CA THR 308 3468 1939 5998 225 -1629 ATOM 2153 C THR 308 10.468 -0.611 54.030 1.000 25.42 ANISOU 2153 C THR 308 2915 2190 4552 453 -626 - 321308 9.523 -0.768 54.787 1.000 30.10 308 4042 3482 3912 614 -217 -2154 0 ATOM THR ANISOU 2154 O THR -217 - 125ATOM 2155 CB THR ANISOU 2155 CB THR 308 12.581 0.531 54.688 1.000 26.09 308 2701 3586 3626 242 -361 --361 -456 308 12.140 0.751 56.028 1.000 32.90 308 4146 4188 4167 504 745 -ATOM 2156 OG1 THR ANISOU 2156 OG1 THR 745 - 495 308 13.577 1.594 54.256 1.000 31.43 308 3193 4702 4047 -577 -132 -538 ATOM 2157 CG2 THR ANISOU 2157 CG2 THR ATOM 2158 N SER 309 10.850 -1.591 53.217 1.000 24.73 ANISOU 2158 N SER 309 2934 2092 4370 94 -574 - 391 2159 CA SER ATOM 309 10.199 -2.897 53.230 1.000 25.19 ANISOU 2159 CA SER -485 451 -230 ATOM 2160 C SER

 309
 10.466
 -3.691
 54.512
 1.000
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 309
 2360
 2888
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 11.565
 -3.621
 55.084
 1.000
 34.54

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 3626
 2131
 7366
 -76
 -1944

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 -844
 -2

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 9.494
 -4.458
 54.961
 1.000
 24.99

 310
 3172
 2459
 3864
 160
 262
 3

 310
 9.651
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 56.125
 1.000
 28.38

 ANISOU 2160 C SER 107 3 5 ATOM 2161 0 SER ANISOU 2161 O SER -1944 - 342162 CB SER ANISOU 2162 CB SER 580 - 366 2163 OG SER ANISOU 2163 OG SER -844 - 2602164 N LYS ANISOU 2164 N LYS 262 366 2165 CA LYS 310 9.651 -5.339 56.125 1.000 28.38 ANISOU 2165 CA LYS 310 4191 3167 3427 764 278 2 310 9.941 -6.768 55.711 1.000 26.07 278 281 2166 C LYS 310 9.941

- 84 -ANISOU 2166 C LYS 310 3371 2687 3846 168 -290 5 7 7 2167 O LYS 310 10.150 -7.684 56.515 1.000 33.48 ANISOU 2167 O LYS 310 5267 3056 4400 -66 -450 1073 MOTA 2168 CB LYS 310 8.299 -5.367 56.858 1.000 37.77 ANISOU 2168 CB LYS 310 5736 4695 3921 299 1818 1 8 310 8.014 -4.214 57.806 1.000 40.55 MOTA 2169 CG LYS ANISOU 2169 CG 310 6395 4716 4295 1525 1524 1 310 6.798 -4.587 58.649 1.000 44.24 LYS 1524 1 0 1 ATOM 2170 CD LYS ANISOU 2170 CD 310 9091 4224 3495 1053 2816 5 310 6.722 -6.109 58.818 1.000 59.12 LYS 2816 5 8 4 ATOM 2171 CE LYS ANISOU 2171 CE 310 9281 4577 8606 766 -82 2 310 6.088 -6.563 60.089 1.000 55.80 LYS -82 2478 ATOM 2172 NZ LYS ANISOU 2172 NZ LYS ATOM 2173 N ALA ANISOU 2173 N ALA ATCM 2174 CA ALA ANISOU 2174 CA ALA MOTA 2175 C ALA ANISOU 2175 C ALA ATOM 2176 CB ALA311 2407 2878 5329 -355 542 -672 501 -6.477 10.237 44.256 1.000 15.66 502 -9.349 16.189 51.010 1.000 19.26 ANISOU 2176 CB ALA2177 OW ATOM HOH ATOM 2178 OW HOH 503 -1.489 3.653 34.560 1.000 15.78 504 -10.499 18.731 50.182 1.000 16.19 505 -8.612 16.958 47.640 1.000 17.30 ATOM 2179 OW HOH 2180 OW MOTA HOH ATOM 2181 OW HOH 506 -10.255 20.839 42.881 1.000 19.05 507 2.096 1.076 32.810 1.000 29.32 MOTA 2182 OW HOH 2183 OW MOTA HOH MOTA 2184 OW HOH 508 -0.284 4.743 41.885 1.000 13.93 MOTA 2185 OW 509 -8.525 18.553 42.416 1.000 21.33 HOH ATOM 2186 OW нон 510 3.165 2.604 43.488 1.000 24.59 MOTA 2187 OW HOH 511 -6.282 19.386 52.341 1.000 18.98 ATOM 2188 OW нон 512 -6.826 24.638 46.833 1.000 21.77 ATOM 2189 OW HOH 513 10.510 -4.344 46.092 1.000 25.88 ATOM 2190 OW 514 -0.806 16.964 40.372 1.000 16.54 HOH ATOM 2191 OW 515 -1.269 18.855 HOH 42.411 1.000 15.76 ATOM 2192 OW HOH 516 14.277 -5.146 40.175 1.000 15.53 ATOM 2193 OW 517 -0.123 21.538 40.640 1.000 17.22 HOH 518 13.131 -0.967 51.791 1.000 17.22 519 11.009 2.875 45.599 1.000 20.20 520 5.789 13.543 45.996 1.000 17.36 521 2.168 19.767 55.925 1.000 20.41 522 8.487 15.960 34.949 1.000 15.40 ATOM 2194 OW HOH ATOM 2195 OW HOH ATOM 2196 OW HOH 2197 OW ATOM HOH ATOM 2198 OW HOH 15.960 34.949 1.000 15.40 523 10.794 12.697 29.921 1.000 19.99 ATOM 2199 OW НОН ATOM 524 -11.722 19.112 44.516 1.000 19.82 525 1.672 -2.081 35.124 1.000 16.29 2200 OW нон ATOM. 2201 OW HOH 35.124 1.000 16.29 32.342 1.000 20.37 -2.081 ATOM 2202 OW HOH 526 9.651 15.283 ATOM 2203 OW HOH 527 28.749 31.187 52.019 1.000 18.53 32.041 1.000 19.60 2204 OW ATOM нон 528 15.326 11.252 2205 OW ATOMHOH 529 26.897 26.984 52.035 1.000 19.86 ATOM 2206 OW НОН 530 13.528 11.592 50.915 1.000 16.17 ATOM 2207 OW 531 25.631 НОН 32.409 52.682 1.000 19.20 ATOM 2208 OW 532 18.287 HOH6.835 52.185 1.000 18.49 MOTA 2209 OW 533 12.635 нон 29.035 39.395 1.000 18.09 ATOM 2210 OW 534 10.797 HOH 31.963 45.659 1.000 20.66 MOTA 2211 OW 535 10.167 НОН 33.567 1.000 19.12 24.890 MOTA 2212 OW 536 23.530 HOH 24.122 58.531 1.000 20.39 2213 OW ATOM НОН 537 23.358 12.639 35.292 1.000 22.61 ATOM 2214 OW HOH 538 25.879 28.699 50.264 1.000 19.44 2215 OW ATOM HOH 539 11.674 16.559 30.502 1.000 18.57 2216 OW ATOM HOH 540 18.515 27.775 40.042 1.000 22.23

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MOTA 2217 OW нон 541 21.233 20.367 33.996 1.000 21.45 542 22.826 MOTA 2218 OW нон 32.643 53.094 1.000 19.38 ATOM 2219 OW нон 543 19.670 22.387 35.310 1.000 20.05 ATOM 2220 OW нон 544 -13.591 21.996 61.494 1.000 49.93 ATOM 2221 OW нон 545 21.295 11.783 55.080 1.000 20.04 ATOM 2222 OW нон 546 5.431 2.533 51.677 1.000 28.11 ATOM 2223 OW НОН 547 17.311 25.489 32.148 1.000 24.38 ATOM 2224 OW HOH 548 17.427 7.744 33.008 1.000 20.78 ATOM 2225 OW HOH 549 11.656 23.874 58.194 1.000 23.39 ATOM 2226 OW HOH 550 8.037 14.987 53.326 1.000 33.52 ATOM 2227 OW нон 551 1.354 14.574 33.889 1.000 21.05 ATOM 2228 OW НОН 552 11.203 20.116 63.686 1.000 24.59 2229 OW ATOM HOH 553 2.671 21.240 34.245 1.000 34.51 2230 OW 554 6.339 19.832 ATOM HOH 30.751 1.000 26.36 2231 OW ATOM нон 555 26.611 24.519 55.570 1.000 21.22 2232 OW ATOM нон 556 27.669 17.156 53.039 1.000 25.86 2233 OW ATOM HOH 557 -14.392 19.977 44.154 1.000 25.03 MOTA 2234 OW нон 558 14.828 32.652 51.443 1.000 25.23 MOTA 2235 OW нон 559 17.937 54.915 1.000 20.59 31.499 1.000 24.65 7.207 560 10.729 ATOM 2236 OW нон -8.875 2237 OW ATOM нон 561 6.455 2.298 42.613 1.000 22.74 ATOM 2238 OW нон 562 13.784 31.245 44.166 1.000 27.75 ATOM 2239 OW нон 563 17.292 53.556 1.000 25.28 49.697 1.000 23.33 33.470 ATOM 2240 OW нон 564 11.210 1.109 ATOM 2241 OW HOH 565 -11.339 25.246 41.370 1.000 26.08 566 20.363 ATOM 2242 OW нон -8.375 38.242 1.000 30.07 ATOM 2243 OW нон 567 3.890 24.604 35.837 1.000 25.86 568 5.334 ATOM 2244 OW HOH 11.875 43.937 1.000 25.45 ATOM 2245 OW HOH 569 7.861 22.385 64.046 1.000 28.98 ATOM 2246 OW HOH 570 7.754 -1.508 30.848 1.000 24.72 ATOM 2247 OW нон 571 6.297 3.583 28.471 1.000 33.06 ATOM 2248 OW HOH 572 -15.790 28.800 51.855 1.000 30.09 MOTA 2249 OW нон 573 -5.388 20.310 38.883 1.000 23.64 MOTA 2250 OW нон 574 17.657 21.059 29.053 1.000 24.31 MOTA 2251 OW нон 575 8.763 20.920 66.102 1.000 24.81 58.357 1.000 25.12 ATOM 2252 OW НОН 576 10.135 27.617 577 7.795 ATOM 2253 OW нон 1.060 29.730 1.000 29.00 578 22.601 ATOM 2254 OW 61.946 1.000 28.66 HOH 19.580 нон ATOM 2255 OW 579 8.859 27.898 1.000 26.12 4.744 ATOM 2256 OW HOH 580 4.937 48.882 1.000 26.29 3.932 35.057 1.000 23.31 64.719 1.000 54.01 52.106 1.000 27.23 29.292 1.000 26.60 ATOM 2257 OW HOH 581 17.096 5.891 582 -16.337 31.047 583 7.652 24.826 584 7.174 24.915 585 23.452 10.614 ATOM 2258 OW HOH MOTA 2259 OW HOH MOTA 2260 OW нон ATOM 2261 OW HOH 55.439 1.000 26.42 ATOM 2262 OW 586 12.640 26.413 21.166 HOH 58.676 1.000 27.15 ATOM 2263 OW HOH 587 6.204 62.094 1.000 24.65 37.616 1.000 19.92 45.738 1.000 38.29 45.065 1.000 30.46 36.120 1.000 27.12 ATOM 2264 OW HOH 588 2.385 0.810 ATOM 589 32.930 28.236 590 -12.045 28.716 2265 OW HOH ATOM 2266 OW HOH ATOM 2267 OW нон 591 0.219 13.612 ATOM 2268 OW нон 592 -2.525 43.344 1.000 26.67 3.881 MOTA 2269 OW HOH 593 7.533 13.297 48.055 1.000 19.59 ATOM 2270 OW нон 594 -1.575 28.355 42.057 1.000 25.53 MOTA 2271 OW -1.188 -7.000 нон 595 11.209 46.425 1.000 22.12 ATOM 2272 OW HOH 596 5..684 28.451 1.000 27.97 ATOM 2273 OW HOH 597 28.868 19.406 51.825 1.000 27.72 ATOM 2274 OW 598 13.432 HOH 57.904 1.000 31.12 2.493 ATOM 2275 OW HOH 599 8.196 7.483 27.148 1.000 29.99 ATOM 2276 OW НОН 600 20.809 19.088 63.369 1.000 36.86 2277 OW MOTA нон 601 21.352 10.656 34.614 1.000 30.60

- 86 -ATOM 2278 OW HOH 602 2.891 7.196 30.899 1.000 25.41 2279 OW ATOM HOH 603 8.260 26.496 34.561 1.000 35.71 ATOM 2280 OW нон 604 22.300 13.959 35.750 31.378 1.000 32.53 ATOM 2281 OW НОН 605 15.689 48.870 1.000 31.17 MOTA 2282 OW HOH 606 7.219 15.638 30.914 1.000 27.80 MOTA 2283 OW HOH 607 -3.237 14.604 47.092 1.000 20.96 ATOM 2284 OW HOH 608 17.543 10.581 33.561 1.000 23.51 ATOM 2285 OW HOH 609 -1.899 36.370 44.261 1.000 32.64 ATOM 2286 OW НОН 610 26.095 14.431 43.803 1.000 19.19 2287 OW ATOM 611 27.664 HOH 13.183 41.954 1.000 26.48 MOTA 2288 OW HOH 612 4.302 34.604 49.981 1.000 24.70 MOTA 2289 OW HOH 613 -15.580 27.012 46.728 1.000 42.45 50.347 1.000 23.78 нон ATOM 2290 OW 614 1.615 35.544 ATOM 2291 OW HOH 615 -10.137 34.259 49.033 1.000 23.94 ATOM 2292 OW 57.657 1.000 39.32 HOH 616 26.084 6.502 ATOM 2293 OW HOH 617 -15.962 20.656 46.340 1.000 25.74 MOTA 2294 OW нон 618 6.113 29.517 40.143 1.000 29.43 ATOM 2295 OW НОН 619 19.797 4.627 51.313 1.000 27.15 ATOM 2296 OW НОН 620 -1.748 48.716 1.000 21.83 11.315 MOTA 2297 OW HOH 621 11.099 34.289 44.259 1.000 27.15 MOTA 2298 OW HOH 622 28.352 14.351 37.877 1.000 41.48 ATOM 2299 OW HOH 623 -2.826 36.968 57.149 1.000 32.75 2300 OW ATOM 624 16.983 625 16.780 HOH 9.258 29.962 1.000 32.82 ATOM 2301 OW HOH 29.213 38.384 1.000 27.96 ATOM 2302 OW HOH 626 1.632 17.213 33.689 1.000 23.17 ATOM 2303 OW 627 33.536 HOH 23.640 45.028 1.000 41.91 ATOM 2304 OW нон 628 23.821 6.059 50.174 1.000 34.22 MOTA 2305 OW 629 3.482 HOH 2.785 46.751 1.000 39.07 2306 OW MOTA HOH 630 20.218 24.803 60.918 1.000 50.12 2307 OW ATOM HOH 631 3.366 16.272 30.698 1.000 31.50 ATOM 2308 OW HOH 632 18.871 11.791 25.782 31.384 1.000 30.78 ATOM 2309 OW HOH 633 4.455 58.823 1.000 32.14 MOTA 2310 OW HOH 634 24.721 5.202 40.319 1.000 40.13 MOTA 2311 OW НОН 635 19.623 35.238 43.466 1.000 50.48 ATOM 2312 OW НОН 636 22.789 60.797 1.000 26.58 26.242 ATOM 2313 OW HOH 637 7.008 -4.809 54.039 1.000 33.89 ATOM 2314 OW HOH 638 -15.821 18.362 42.559 1.000 29.61 ATOM 2315 OW HOH 639 -11.847 15.711 52.841 1.000 25.21 ATOM 2316 OW HOH 640 -1.948 13.411 35.401 1.000 30.41 ATOM 2317 OW HOH 641 -14.293 21.937 42.145 1.000 27.58 ATOM 2318 OW HOH 642 18.216 20.839 66.863 1.000 31.23 ATOM 2319 OW HOH 643 9.836 36.288 48.178 1.000 44.21 ATOM 2320 OW HOH 644 3.510 16.168 66.253 1.000 33.82 ATOM 2321 OW 645 7.571 HOH 33.398 41.687 1.000 37.96 MOTA 2322 OW HOH 646 0.780 21.844 36.729 1.000 31.71 ATOM 2323 OW HOH 647 21.244 -2.321 35.579 1.000 32.40 ATOM 2324 OW HOH 648 3.027 25.244 69.907 1.000 36.84 ATOM 2325 OW HOH 649 1.129 25.273 66.516 1.000 35.42 ATOM 2325 OW HOH 650 14.646 7.560 60.327 1.000 46.42 ATOM 2327 OW HOH 651 -8.287 26.381 37.998 1.000 29.17 ATOM 2328 OW HOH 652 10.153 23.548 67.703 1.000 31.50 ATOM 2329 OW нон 653 28.906 22.258 38.969 1.000 32.66 MOTA 2330 OW 654 13.568 HOH -4.482 31.517 1.000 26.94 MOTA 2331 OW 655 -12.635 17.106 HOH 55.637 1.000 26.85 ATOM 2332 OW HOH. 656 2.698 5.770 50.702 1.000 29.05 ATOM 2333 OW 657 -1.384 HOH 7.487 46.512 1.000 36.52 ATOM 2334 OW HOH 658 3.880 19.246 31.498 1.000 31.50 MOTA 2335 OW HOH 659 -1.400 31.406 64.001 1.000 56.62 ATOM 2336 OW нон 660 11.416 23.260 65.229 1.000 32.69 ATOM 2337 OW нон 661 15.994 14.673 25.680 1.000 36.46 MOTA 2338 OW HOH 662 28.572 21.242 53.423 1.000 39.06

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ATOM	2339 OW	НОН	663 19.354	0.465		1.000 44.56	
ATOM ATOM	2340 OW 2341 OW	нон	664 24.969	27.026	38.838		
ATOM	2341 OW 2342 OW	нон нон	665 24.294 666 19.540	7.488	55.914		
ATOM	2343 OW	нон	667 -9.236	7.882	31.178		
ATOM	2344 OW	нон	668 2.098	32.988	57.241		
ATOM	2345 OW	нон	669 11.390	18.351 3.245	67.496		
ATOM	2346 OW	нон	670 -21.413	3.243	56.270 52.026		
ATOM	2347 OW	- НОН	671 -14.575		55.240	1.000 44.66 1.000 30.91	
ATOM	2348 OW	нон	672 32.112	25.958	43.051		
MOTA	2349 OW	HOH	673 -15.050	31.151	53.232		
ATOM	2350 OW	HOH	674 2.941	-1.607	30.245	1.000 34.63	
MOTA	2351 OW	нон	675 26.951	14.544	34.757	1.000 49.17	
ATOM	2352 OW	нон	676 14.707	30.669	39.386	1.000 30.55	
ATOM ATOM	2353 OW 2354 OW	нон нон	677 5.203 678 14.151	18.009	68.080	1.000 43.41	
ATOM	2355 OW	HOH	678 14.151 679 24.470	7.965 24.261	26.591	1.000 38.80	
ATOM	2356 OW	НОН	680 17.540	2.410	41.443	1.000 31.28 1.000 34.31	
ATOM	2357 OW	нон	681 25.992	20.593	34.326	1.000 34.31	
ATOM	2358 OW	HOH	682 13.802	35.357	44.421	1.000 33.00	
ATOM	2359 OW	HOH	683 1.087	2.355	45.456	1.000 35.39	
ATOM	2360 OW	нон	684 22.443	34.538	42.053	1.000 33.55	
ATOM	2361 OW	нон	685 4.419	4.720	27.356	1.000 48.02	
ATOM ATOM	2362 OW 2363 OW	НОН	686 -15.830	34.507	51.877	1.000 50.63	
ATOM	2364 OW	нон нон	687 -15.217 688 36.808		48.887	1.000 33.54	
ATOM	2365 OW	HOH	689 3.756	21.183 1.312	46.206	1.000 44.97 1.000 35.16	
ATOM	2366 OW	нон	690 18.802	13.646	27.901	1.000 35.16	
ATOM	2367 OW	нон	691 6.997	17.521	29.313	1.000 30.08	
ATOM	2368 OW	HOH	692 13.725	16.327	69.105	1.000 36.97	
ATOM	2369 OW	нон	693 22.369	22.161	60.503	1.000 44.09	
ATOM	2370 OW	нон	694 -5.429	31.620	42.219	1.000 33.40	
ATOM ATOM	2371 OW 2372 OW	НОН	695 19.351	23.082	30.744	1.000 34.21	
ATOM	2372 OW 2373 OW	нон нон	696 6.897 697 28.700	22.414	29.376	1.000 36.59	
ATOM	2374 OW	HOH	698 3.224	7.809 0.679	57.304 39.819	1.000 38.35	
MOTA	2375 OW	нон	699 -4.634	33.717	62.593	1.000 24.13 1.000 32.26	
MOTA	2376 OW	нон	700 32.423	17.018	43.200	1.000 43.20	
ATOM	2377 OW	HOH	701 12.119	25.228	68.342	1.000 39.95	
ATOM	2378 OW	нон	702 9.307	16.477	28.976	1.000 31.75	
ATOM ATOM	2379 OW	нон	703 -11.313		46.117	1.000 49.40	
ATOM	2380 OW 2381 OW	нон нон	704 7.774	31.390	65.371	1.000 39.12	
ATOM	2382 OW	НОН	705 24.764 706 -22.095		36.802	1.000 38.55	
ATOM	2383 OW	нон	707 14.509	9.840		1.000 36.71 1.000 50.38	
ATOM	2384 OW	нон	708 -10.129		42.036	1.000 30.38	
ATOM	2385 OW	HOH	709 29.011	34.910		1.000 35.29	
ATOM	2386 OW	HOH	710 15.822	31.612		1.000 33.61	
ATOM	2387 OW	нон	711 -1.996	17.676	33.645	1.000 49.57	
ATOM ATOM	2388 OW	нон	712 10.216	17.748		1.000 41.04	
ATOM	2389 OW 2390 OW	HOH	713 23.535	29.642		1.000 43.47	
ATOM	2391 OW	нон нон	714 20.488 715 11.411	-7.214		1.000 45.99	
ATOM	2392 OW	НОН	715 11.411 716 19.329	10.149 -4.258		1.000 41.63	
ATOM	2393 OW	нон	717 13.688	26.799		1.000 42.50 1.000 43.74	
ATOM	2394 OW	нон	718 -10.751			1.000 43.74	
ATOM	2395 OW	нон	719 13.800	18.258		1.000 34.54	
ATOM	2396 OW	нон	720 17.151	5.815		1.000 40.80	
MOTA	2397 OW	нон	721 0.000	0.000	36.691	0.330 27.42	
ATOM ATOM	2398 OW 2399 OW	HOH	722 0.000	0.000		0.330 37.77	
AION	2333 UW	нон	723 15.314	7.549	28.791	1.000 36.24	

ATOM	2400) OW	НОН	724	-1.663	19.944	39.196	1.000	33.87
ATOM	2401	L OW	НОН	725	19.289	24.195	33.321		
ATOM	2402	WO S	HOH	726	0.000	0.000	31.798		
ATOM	2403	WO	HOH	727	-1.223	38.165	59.229		
ATOM	2404	. OW	HOH	728	22.035	38.254	45.742		
ATOM	2405	OW	HOH	729	28.388	16.248	63.044		
ATOM	2406	OW	HOH	730	0.000	0.000	45.995	0.330	36.14
ATOM	2407	OW	HOH	731	2.984	29.007	40.091	1.000	36.08
ATOM	2408	OW	HOH	732	5.297	15.835	27.318	1.000	41.53
ATOM	2409		HOH	733	17.347	10.778	27.373	1.000	35.27
ATOM	2410		HOH	734	29.417	14.607	53.127	1.000	40.12
ATOM	2411		нон	735	4.222	-8.636	27.012	1.000	35.22
ATOM	2412		нон	736	-9.949	17.712	62.813	1.000	34.43
ATOM	2413		HOH	737	13.960	-10.203	55.259	1.000	31.79
ATOM	2414		НОН	738	11.831	-1.522	49.308	1.000	25.22
ATOM	2415	OW	HOH	739	2.896	4.247	29.596	1.000	38.64
ATOM	2416		нон	740	10.959	13.759	25.528	1.000	61.86
MOTA	2417	OM	HOH	741	0.864	17.227	30.557	1.000	50.71
ATOM	2418	OW	HOH	742	31.755	18.949	52.065	1.000	40.48
ATOM	2419		HOH	743	21.678	-0.485	28.218	1.000	43.23
ATOM	2420		нон	744	10.583	16.397	75.211	1.000	45.04
ATOM	2421		HOH	745	7.480	7.996	78.287	1.000	57.64
ATOM	2422	OM	HOH	746	24.067	35.122	40.297	1.000	41.95
ATOM	2423	OW	HOH	747	7.804	10.269	78.332	1.000	49.63
ATOM	2424	OW	HOH	748	22.131	40.645	45.806	1.000	49.69
ATOM	2425	OM	HOH	749	14.850	-4.647	33.872	1.000	42.88
ATOM	2426	OW	HOH	750	-12.930	32.504	55.211	1.000	37.15
ATOM	2427	OW	HOH	751	-4.832	35.986	43.333	1.000	44.39
ATOM	2428	OW	НОН	752	19.834	33.566	56.449	1.000	31.56
ATOM	2429	OW	НОН	753	3.363	22.310	29.844	1.000	42.02
ATOM	2430	OW	HOH	754	25.594	4.030	34.174	1.000	51.90
ATOM	2431	OM	нон	755	28.036	35.859	46.448	1.000	39.50
ATOM	2432	OW	HOH	756	-12.951	16.294	61.787	1.000	40.94
ATOM	2433	OW	HOH	757	-10.870	26.452	38.737	1.000	44.85
ATOM	2434	OW	HOH	758	13.216	12.896	70.729	1.000	63.42
ATOM		OW	нон	7 59	-0.403	21.161	74.990	1.000	38.96
ATOM	2436		HOH		-7.025	32.526	64.316	1.000	39.64
ATOM	2437	OW	HOH		-15.459	19.739	58.090	1.000	40.84
ATOM	2438	OW	НОН	762	-4.964	36.577	59.068	1.000	48.64
ATOM	2439		HOH	763	26.807	35.717	50.036	1.000	43.54
ATOM		OM	нон		19.542	7.083	65.538	1.000	41.41
ATOM		OM	HOH	765	3.709	35.837	42.709	1.000	33.78
ATOM		OW	НОН	766	0.431	33.688	40.172	1.000	36.91
ATOM		OW	нон	767	18.620	5.064	64.617	1.000	45.76
ATOM	2444	OM	НОН	768	35.526	19.792	41.322	1.000	52.54
ATOM	2445	OM	нон	769	19.671	7.789	67.717	1.000	
ATOM	2446	OW	HOH	770	3.562	12.048	26.149	1.000	
ATOM	2447	OW	HOH	771	20.245	35.637	53.927	1.000	52.16
ATOM		OW	HOH	772	-20.588	25.640	61.573	1.000	58.60
ATOM	2449	OW	HOH	773	1.556	37.342	52.171	1.000	36.23
ATOM	2450	OW	нон	774	8.340	0.668	49.382	1.0001	
ATOM	2451	OW	НОН	775	27.160	2.372	34.466	1.000	59.84
MOTA	2452	OM	НОН		6.575	19.271	25.545	1.000	36.68
								-	

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MOTA	2453	OW	нон	777	-17.605	29.205	62.661	1.000	56.83
MOTA	2454	OW	нон	778	7.616	6.902	24.722		
MOTA	2455	OW	HOH	779	19.749	10.700	68.006	1.000	65.22
ATOM	2456	W	НОН	780	7.281	-5.270	50.090	1.000	50.00
ATOM	2457	W	НОН	781	-6.809	28.483	40.515	1.000	50.00
ATOM	2458	W	нон	782	9.990	17.263	38.636	1.000	50.00
ATOM	2459	W	нон	783	5.767	-2.331	28.939	1.000	50.00
MOTA	2460	W	HOH	784	11.694	-0.118	24.984	1.000	50.00
ATOM	2461	W	HOH	785	24.442	7.952	47.994	1.000	50.00
ATOM	2462	W	HOH	786	14.251	36.889	46.491	1.000	50.00
ATOM	2463	W	HOH	787	5.759	26.477	33.851	1.000	50.00
ATOM	2464	W	HOH	788	-11.816	22.606	40.795	1.000	50.00
ATOM	2465	W	HOH	789	-2.531	5.579	45.829	1.000	50.00
MOTA	2466	W	HOH	790	-13.002	32.034	46.612	1.000	50.00
ATOM	2467	W	HOH	791	2.230	3.555	48.985	1.000	50.00
MOTA	2468	W	HOH	792	9.397	13.464	28.121	1.000	50.00
ATOM	2469	W	HOH	793	28.257	10.442	42.781	1.000	50.00
ATOM	2470	W	HOH	794	4.652	17.944	59.241	1.000	50.00
MOTA	2471	W	HOH	795	5.977	15.287	79.554	1.000	50.00
ATOM	2472	W	HOH	796	30.501	11.852	47.616	1.000	50.00
MOTA	2473	W	HOH	7 97	5.625	14.258	54.367	1.000	50.00
ATOM	2474	W	HOH	798	23.942	20.228	33.277	1.000	50.00
MOTA	2475	W	HOH	799	10.164	14.642	58.997	1.000	50.00
MOTA	2476	M	HOH	800	7.807	31.943	52.999	1.000	50.00
ATOM	2477	W	HOH	801	23.377	9.361	34.817	1.000	50.00
ATOM	2478	W	HOH	802	21.193	9.722	32.004	1.000	50.00
ATOM	2479	W	HOH	803	34.928	14.644	46.038	1.000	50.00
ATOM	2480	W	HOH	804	29.073	16.684	34.445	1.000	50.00
MOTA	2481	W	HOH	805	7.008	-2.049	51.872	1.000	50.00
ATOM	2482	W	HOH	806	25.363	7.860	45.531	1.000	50.00
ATOM	2483	W	HOH	807	30.704	8.207	55.971	1.000	50.00
ATOM	2484	W	нон	808	33.072	24.900	40.599	1.000	50.00
ATOM	2485	W	нон	809	-15.577	19.225	63.152	1.000	50.00
MOTA	2486	W	HOH	810	6.072	18.137	23.603	1.000	50.00
ATOM	2487	W	нон	811	-7.214	39.940	55.639	1.000	50.00
ATOM	2488	W	нон	812	5.509	18.517	74.919	1.000	50.00
ATOM	2489	W	нон	813	33.845	9.908	56.672	1.000	50.00
ATOM	2490	W	HOH	814	0.421	35.779	42.931	1.000	50.00
ATOM	2491	M	нон	815	35.282	21.705	48.656	1.000	50.00
MOTA	2492	M	HOH	816	39.344	22.173		1.000	
ATOM	2493	W	HOH	817	-5.192	39.820			50.00
MOTA	2494	M	HOH	818	30.199	13.039	33.383		50.00
ATOM	2495	M	нон	819	-4.860	36.454	61.731		50.00
ATOM	2496	W	нон	820	-14.599	17.407	58.382		50.00
ATOM	2497	W	НОН	821	1.340	-0.111	41.711	0.500	50.00
MOTA	2498	W	НОН			23.218	52.108	1.000	50.00
MOTA	2499	W	НОН	823	32.136	12.571	52.190	1.000	50.00
MOTA	2500	W	HOH	824	13.525	-6.549	29.838	1.000	50.00
ATOM	2501	W	нон	825	6.072	-4.141	27.534	1.000	

STRUCTURE B

ATOM 8 ANISOU 8 ATOM 9 ANISOU 9 ATOM 10 ANISOU 10 ATOM 11 ANISOU 11 ATOM 12 ANISOU 12 ATOM 13 ANISOU 13 ATOM 14 ANISOU 14 ANISOU 15 ANISOU 15 ANISOU 15 ATOM 16 ANISOU 17 ANISOU 17 ANISOU 17 ANISOU 17 ANISOU 17 ANISOU 17 ANISOU 19 ANISOU 19 ANISOU 20 ANISOU 20 ATOM 21 ANISOU 20 ATOM 21 ANISOU 21 ATOM 22 ANISOU 22 ATOM 23 ANISOU 22 ATOM 23 ANISOU 23 ANISOU 24 ANISOU 24 ANISOU 25 ATOM 26 ANISOU 26 ATOM 27 ANISOU 27 ANISOU 27 ANISOU 28	METTTTTTTTTTTTPPPPPPPPPPPPPPPPPPPPPPPPP	1111111111111112222222222222222233333333	31.03 0 6 2 8 9 0 0 6 5 9 6 9 5 3 5 2 4 3 1 0 4 4 7 2 9 2 3 2 6 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	113323133131313131313131313131313131313	59.663 59.663 59.556 5094 58.379 4489 60.597 3807 60.421 3753 61.414 4495 62.758 3989 61.315 7630 60.553 3939	1.000 5 0.96 1113 -2217 - 5 5 4 1.000 5 1.63 691 -1891 1 6 9 1.000 4 0.50 833 -1535 - 4 6 0 1.000 45.32 -239 -653 - 1702 1.000 52.14 287 -2128 - 6 3 1.000 52.92 1417 -4224 5 1 9 1.000 57.78 34 -1912 - 8 1 1 1.000 5 4.62 137 -2012 - 6 1 7 1.000 43.52 474 -2350 4 7 1.000 41.69 -309 -2603 - 3 1 1.000 37.89 -304 -3473 2 6 6 1.000 39.59 15 -3218 5 8 9 1.000 45.10 -553 -1950 - 6 2 5 1.000 42.05 -465 -3788 1 4 5 1.000 33.84 -59 -1682 - 1 2 2 1.000 29.25 658 -390 - 6 1 5 1.000 29.41 907 -2076 - 2 8 4 1.000 28.55 597 -1006 - 3 9 0 1.000 36.51 -791 -1996 5 2 1.000 42.45 -920 -1251 3 8 3 1.000 50.26 -602 -733 - 3 3 3 1.000 29.01 738 -1079 9 9 1.000 35.82 390 524 -1246 1.000 24.98 542 -2040 - 9 8 6 1.000 23.97 344 -1563 - 3 7 5 1.000 26.77 651 -988 -9 2 3 1.000 26.40 533 -573 - 1570
ATOM 27 ANISOU 27 ATOM 28 ANISOU 28 ATOM 29 ANISOU 29 ATOM 30 ANISOU 30	OG1 THR OG1 THR CG2 THR	4 4 4	28.050 3398 26.429	19.484 2812 20.942	61.551 6184 60.663 4967 59.097 2374 57.980 2902	1.000 32.62 195 -2081 -1134 1.000 26.40

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N VAL 5
CA VAL 5
CA VAL 5
ANISOU 31
                           2505
                                    2021
                                            1508 -613 -630 - 162
                           23.211 19.385 58.211 1.000 14.80
ATOM
      3 2
ANISOU 32
                                    1893 1266 -594 -473 - 87
19.402 58.606 1.000 16.09
                           2463
ATOM
       3 3
             CB VAL 5
                           21.742
             CB VAL 5
ANISOU 33
                                   1881 1757 -412 -406 5 0 2
19.846 57.447 1.000 14.91
                           2476
             CG1 VAL 5
ATOM
       34
                           20.855
                                   1859 1337 9 -102 19
17.994 59.074 1.000 21.15
ANISOU 34
             CG1 VAL 5
                           2468
                                            1337 9 -102 197
       35
            CG2 VAL 5
                           21.310
ANISOU 35
             CG2 VAL 5
                           3015 2345 2677 -700 -4181
23.639 20.762 57.694 1.000 17.70
                                                    -700 -418 1198
ATOM 36 C VAL 5
ANISOU 36 C VAL 5
                           2893
                                                    -1137 -713 1 0 3
                                    2085
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                           2893 2085 1/49 -113/-/13 1
23.532 21.759 58.419 1.000 17.35
           O VAL 5
      37
ATOM
ANISOU 37
           O VAL 5
                           2566
                                    1978
           N PRO 6 24.150 20.845 56.479 1.000 13.23
                                            2050 -698 -650 1 0 5
ATOM
      38
           N PRO 6 1334
ANISOU 38
                                    1597
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                                                    -162 -668 4 0 9
       39 CD PRO 6 24.302 19.770 55.484 1.000 15.56
ATOM
ANISOU 39
           CD PRO 6 1887
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                                            2176
                                                    -309 -383 2 7 7
MOTA
      40
            CA PRO 6 24.667 22.137 56.005 1.000 14.49
ANISOU 40
            CA PRO 6 1332
                                    1740
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                                                    -218 -536 5 2 2
            CB PRO 6 25.571 21.722 54.847 1.000 18.21
ATOM
       41
             CB PRO 6 2294
ANISOU 41
                                    1740
                                            2886
                                                    -224 130 434
      42
            CG PRO 6 25.132 20.378 54.409 1.000 20.37 CG PRO 6 2708 2632 2399 -1078 38 - 6
ATOM
ANISOU 42
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            C PRO 6 23.576 23.091 55.510 1.000 14.59
C PRO 6 1388 1712 2443 -406 -786 69
O PRO 6 22.408 22.743 55.295 1.000 13.06
O PRO 6 1298 1547 2118 -283 -596 1
N THR 7 24.048 24.326 55.313 1.000 14.56
N THR 7 1393 1678 2463 -380 -565 58
CA THR 7 23.288 25.428 54.771 1.000 13.28
MOTA
       43
ANISOU 43
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ATOM
       44
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1393 1678 2463 -380 -565 5

23.288 25.428 54.771 1.000 13.28

1463 1584 1998 -469 -734 4

23.121 26.572 55.799 1.000 14.44

1927 1652 1905 -348 -1257
ANISOU 44
                                                    -283 -596 1 5
       45
MOTA
ANISOU 45
                                                     -380 -565 5 8 7
ATOM
       46
            CA THR
ANISOU 46
            CA
                 THR
                                                     -469 -734 4 4 0
ATOM
      47
            CB
                 THR
ANISOU 47
            C3
                 THR
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            OG1 THR
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MOTA
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ANISOU 48
            OG1 THR 7
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            CG2 THR
ATOM
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            CG2 THR
ANISOU 49
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ATOM
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ANISOU 50 C
                 THR 7
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      51 O THR 7
MOTA
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ANISOU 51
            O THR 7
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                                                    -641 -840 9 7 5
ATOM
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           N PHE 8
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ANISOU 52
           N PHE 8
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ATOM
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ANISOU 53
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ATOM
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ATOM
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ANISOU 55
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ATOM
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ANISOU 56
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MOTA
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            CD2 PHE
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ANISOU 57
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ATOM
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ANISOU 58
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ATOM
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ANISOU 59
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MOTA
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                PHE 8
PHE 8
PHE 8
ANISOU 60
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ATOM .
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ATOM
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MOTA
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ATOM
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ANISOU 91
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WO 99/33994			٠	PCT/GB98/03860
		- 93 -		
ANISOU 92 ATOM 93 ANISOU 93 ATOM 94 ANISOU 94 ATOM 95 ANISOU 95 ATOM 96 ANISOU 96 ATOM 97 ANISOU 97 ANISOU 97	CA LEU 13 CB LEU 13 CB LEU 13 CG LEU 13 CG LEU 13 CD1 LEU 13 CD1 LEU 13 CD2 LEU 13 C LEU 13	-93- 1734 1873 24.003 27.248 2205 1838 24.154 26.554 1913 1803 22.934 25.680 2174 1817 25.411 25.690 2119 2043 24.876 28.626 2510 2062	1713 44.620 1795 45.967 1799 46.193 1766 46.067 2502 42.725 1710	-140 -170 4 9 6 1.000 15.37 -375 -149 4 6 5 1.000 14.52 -280 -204 4 4 2 1.000 15.15 -433 185 1 7 5 1.000 17.54 -38 -419 2 7 0 1.000 16.54 -222 -93 5 6 5
ATOM 98 ANISOU 98 ATOM 99 ANISOU 99 ATOM 100 ANISOU 100 ATOM 101 ANISOU 101	O LEU 13 O LEU 13 N GLN 14 N GLN 14 CA GLN 14 CA GLN 14 CB GLN 14 CB GLN 14	25.548 28.122 2685 2514 23.945 29.534 1970 2337 23.657 30.015 2761 2404 22.421 30.923	41.821 1748 42.472 2100 41.132 1915 41.130	1.000 18.28 -687 75 259 1.000 16.86 -557 -683 8 3 8 1.000 18.63 -610 -802 5 6 8 1.000 19.39
ATOM 102 ANISOU 102 ATOM 103 ANISOU 103 ATOM 104 ANISOU 104	CG GLN 14 CG GLN 14 CD GLN 14 CD GLN 14 OE1 GLN 14 OE1 GLN 14	3166 2176 21.108 30.250 2879 2383 19.974 31.227 3139 2118 20.177 32.317 3928 2407	2025 41.460 1957 41.766 1897 42.314 3582	-392 -918 9 7 7 1.000 19.00 -209 -725 4 6 0 1.000 18.83 -6 -1229 4 9 4 1.000 26.10 -98 -1172 - 241
ATOM 105 ANISOU 105 ATOM 106 ANISOU 106 ATOM 107 ANISOU 107 ATOM 108	NE2 GLN 14 NE2 GLN 14 C GLN 14 C GLN 14 O GLN 14 O GLN 14 N GLN 15	3226 2458 24.812 30.951 5089 4340	41.411 2340 40.525 2065 39.311 2152	1.000 20.94 -149 -840 4 5 4 1.000 20.40 -795 -712 9 3 7 1.000 30.48 -2337 -898 1 2 1 1
ANISOU 108 ATOM 109 ANISOU 109 ATOM 110 ANISOU 110 ATOM 111 ANISOU 111	N GLN 15 CA GLN 15 CA GLN 15 CB GLN 15 CB GLN 15 CG GLN 15	3252 2452 26.909 32.041 3184 3230 27.288 33.100 2720 3162 26.450 34.358	41.329 2030 40.884 1901 41.920 2551 41.954	1.000 20.35 -1067 -240 4 9 7 1.000 21.88 -1152 -299 7 8 8 1.000 22.20 -1131 -770 6 9 1 1.000 25.73
ATOM 112 ANISOU 112 ATOM 113 ANISOU 113 ATOM 114 ANISOU 114	CG GLN 15 CD GLN 15 CD GLN 15 OE1 GLN 15 OE1 GLN 15 NE2 GLN 15 NE2 GLN 15	4496 2735 26.325 35.021 6010 3945 27.145 34.884 8425 5866 25.255 35.812 7190 5567	2545 43.306 3631 44.225 4378 43.489 6945	-821 -233 1 2 6 9 1.000 3 5 . 7 6 -643 -229 - 1 3 5 1.000 4 9 . 1 3 -2857 -2197 - 5 6 4 1.000 5 1 . 8 5 62 3 0 6 6 1 0 7
ATOM 115 ANISOU 115 ATOM 116 ANISOU 116 ATOM 117 ANISOU 117	C GLN 15 C GLN 15 O GLN 15 O GLN 15 N GLY 16	28.069 31.079 3451 3513 29.177 31.448 3535 4619 27.828 29.794	40.625 2127 40.213 2845 40.891	1.000 23.93 -990 145 8 8 4 1.000 28.95 -899 510 1225 1.000 25.86

ANISOU 118

ANISOU 119

ANISOU 120

ANISOU 121

ANISOU 122

118

119

120

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122

ATOM

ATOM

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4089

28.812

4785

3427

3925

3266

2299

29.741

30.805

29.387

30.234

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3562

3490

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2713

2931

28.979

2457

2671

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4068

2569

3025

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28.727 44.172 1.000 21.73

-66

-39

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1997 5 2 3

923 733

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                                           LEU 17 30.354
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CD1 LEU 17 29.962 32.444 45.305 1.000 29.81
                                           LEU 17 2708
                                CG
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  ANISOU 125 CD1 LEU 17 29.962 32.444 45.305 1.000 29.81 ANISOU 125 CD2 LEU 17 31.808 31.350 43.974 1.000 32.84 ANISOU 126 CD2 LEU 17 2845 3703 5930 -281 1871 2114 ANISOU 127 C LEU 17 29.886 27.456 44.936 1.000 19.36 ANISOU 127 C LEU 17 2081 2819 2455 -239 545 580 ANISOU 128 O LEU 17 28.773 26.920 44.848 1.000 21.11 ATOM 129 N HIS 18 30.838 26.952 45.706 1.000 21.02 ANISOU 129 N HIS 18 30.838 26.952 45.706 1.000 21.02 ANISOU 129 N HIS 18 2124 2752 3109 -314 193 491
ATOM 128 O LEU 17 28.773 26.920 44.848 1.000 21.11

ANISOU 128 O LEU 17 2284 3004 2734 -444 107 1055

ATOM 129 N HIS 18 30.838 26.952 45.706 1.000 21.02

ATOM 130 CA HIS 18 30.678 25.814 46.615 1.000 18.11

ANISOU 130 CA HIS 18 1569 2996 2315 -460 -28 3 6 1

ANISOU 131 CB HIS 18 29.655 26.149 47.702 1.000 21.25

ANISOU 131 CB HIS 18 1731 3332 3010 -45 282 3 5 4

ANISOU 131 CB HIS 18 29.796 27.515 48.283 1.000 23.28

ATOM 132 CG HIS 18 29.796 27.515 48.283 1.000 23.28

ANISOU 132 CG HIS 18 2234 3612 2999 211 -46 -20

ANISOU 133 CD2 HIS 18 28.898 28.535 48.344 1.000 24.53

ANISOU 133 CD2 HIS 18 3112 3479 2728 532 41 440

ANISOU 134 ND1 HIS 18 30.940 27.977 48.895 1.000 26.72

ANISOU 135 CE1 HIS 18 30.756 29.218 49.307 1.000 29.80

ANISOU 135 CE1 HIS 18 4476 3775 3071 -542 -562 2 3 7
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136 NE2 HIS 18 29.524 29.581 48.985 1.000 30.03
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ATOM 136 NE2 HIS 18 29.524 29.581 48.985 1.000 30.03
ANISOU 136 NE2 HIS 18 4752 3282 3377 216 -148 3 3 8
ATOM 137 C HIS 18 30.266 24.528 45.917 1.000 18.57
ANISOU 137 C HIS 18 1943 3084 2028 -951 30 5 9 0
ANISOU 138 O HIS 18 29.594 23.682 46.532 1.000 19.92
ANISOU 138 O HIS 18 1949 3125 2493 -777 -87 9 9 5
ATOM 139 N GLN 19 30.647 24.340 44.658 1.000 19.24
ANISOU 139 N GLN 19 30.647 24.340 44.658 1.000 19.24
ATOM 140 CA GLN 19 30.119 23.206 43.908 1.000 21.51
ANISOU 140 CA GLN 19 30.119 23.206 43.908 1.000 21.51
ATOM 141 CB GLN 19 30.446 23.307 42.406 1.000 22.89
ANISOU 141 CB GLN 19 3231 30.58 2408 -148 463 24 4
ANISOU 142 CG GLN 19 3231 3058 2408 -148 463 2 4 4
ANISOU 142 CG GLN 19 3445 3712 2658 -384 -407 5 6 8
ANISOU 143 CD GLN 19 3439 4722 3832 -252 -988 3 5 7
ATOM 143 CD GLN 19 3439 4722 3832 -252 -988 3 5 7
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 ANISOU 144
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27.621 25.433 42.475 1.000 33.32
                                OE1 GLN
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 ATOM
                    145 NE2 GLN
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 ANISOU 145 NE2 GLN
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21.873 44.485 1.000 20.32
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 ATOM
                   146 C
                                           GLN
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 ANISOU 146 C
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ATOM 147 O GLN 19 29.806

ANISOU 147 O GLN 19 1888

ATOM 148 N ASP 20 31.800

ANISOU 148 N ASP 20 3001
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3507 2645 -773 -507 4 1 5
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ATOM 149 CA ASP 20 32.268
ANISOU 149 CA ASP 20 1707
ATOM 150 CB ASP 20 33.780
ANISOU 150 CB ASP 20 1594
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                                                                                          3811 2774 -327 -58 3
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 ATOM
                    151
                               CG ASP
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                                                                 34.596
                               CG ASP
OD1 ASP
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                                                                 2531 5859 4701 -1208 1213 -1
34.177 19.982 43.457 1.000 33.11
                                                         20
                                                                                                                                  -1208 1213 - 280
 ATOM
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                                                                                                              4640
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 ATOM
                                 OD2 ASP
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- 95 -

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ANISOU 153
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MOTA
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ANISOU 164
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MOTA
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ATOM
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ANISOU 172
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ATOM
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ANISOU 173
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                                1430
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ATOM
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ANISOU 174
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ANISOU 222 O ARG

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CG2 THR 42
N GLU 43
N GLU 43
CA GLU 43
CA GLU 43
C GLU 43
C GLU 43
O GLU 43
O GLU 43
CB GLU 43 ANISOU 336 OG1 THR 42 6998 3682 6912 -3163 -1478 1 7 7 337 8.582 39.253 55.872 1.000 45.59 ANISOU 337 9083 3877 4363 -2166 -1048 238 MOTA 338 35.773 54.862 1.000 31.74 7.573 ANISOU 338 3380 4360 4319 -673 -223 - 782 ATOM 339 CA
ANISOU 339 CA
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ATOM 341 O
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ANISOU 368 CB ALA 47 0.548 31.900 54.191 1.000 23.54
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ATOM 369 C ALA 47 3524 1717 3705 -617 1237 -159
ATOM 370 O ALA 47 2282 2546 2752 -327 19.257
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ANISOU 373 C LYS 48 1.110 31.329 59.322 1.000 20.57
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ANISOU 376 CG LYS 48 1.52 30.758 59.294 1.000 24.61
ANISOU 377 CD LYS 48 1.837 30.575 61.736 1.000 41.45
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ANISOU 379 NZ LYS 48 1.837 30.575 61.736 1.000 41.63
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ANISOU 379 NZ LYS 48 1.625 29.777 62.966 1.000 41.63
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ANISOU 379 NZ LYS 48 1.625 29.777 62.966 1.000 41.63
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ANISOU 382 CB ASP 49 -1.868 34.756 60.611 1.000 23.97
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ANISOU 384 OD1 ASP 49 -1.868 34.756 60.611 1.000 23.97
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ANISOU 384 OD1 AS
   384 OD1 ASP 49 -0.153 34.153 62.143 1.000 30.75
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ANISOU 473
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OE1 GLU
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ATOM
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ANISOU 483 O
               ALA
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ANISOU 484 N
                GLU
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MOTA
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ATOM
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ATOM
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           CA
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ANISOU 514
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 MOTA
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ANISOU 539
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- 108 -550 ATOM VAL 70 -12.042 13.057 48.782 1.000 13.59 С ANISOU 550 VAL 70 1618 1382 2163 -38 MOTA 551 0 VAL 70 $-11.426\ 14.105\ 48.493\ 1.000\ 14.20$ ANISOU 551 0 VAL 70 1748 1685 1964 -265 26 182 MOTA 552 Ν PRO 71 -11.786 12.365 49.898 1.000 14.21 ANISOU 552 NPRO 71 1607 1507 2285 -115 -62 310 MOTA 553 CD PRO 71 -12.432 11.125 50.378 1.000 14.70 ANISOU 553 CD PRO 71 1920 1590 2076 -201 646 4 CAMOTA 554 PRO 71 -10.830 12.919 50.878 1.000 17.41 ANISOU 554 PRO CA71 2429 2008 2178 -522 -342 4 1 8 555 ATOM CB PRO 71 -11.338 12.304 52.193 1.000 20.87 ANISOU 555 CB PRO 71 3768 2082 2081 -743 190 1 4 ATOM 556 CG PRO 71 -11.908 10.989 51.775 1.000 18.28 ANISOU 556 CG PRO 71 3534 1665 1746 -338 781 - 54 ATOM 557 PRO 71 -9.384 12.543 50.619 1.000 17.14 ANISOU 557 PRO 71 2183 2304 2026 -684 -815 4 4 558 ATOM 0 PRO 71 -8.730 11.796 51.330 1.000 20.54 ANISOU 558 0 PRO 71 2745 2610 2448 -87 -404 4 1 4 559 ATOM N 72 THR -8.834 13.111 49.556 1.000 16.59 ANISOU 559 N 72 2156 THR 2046 2103 -235 -508 - 17 ATOM 560 CA THR 72 -7.496 12.818 49.090 1.000 17.43 ANISOU 560 CA THR 72 2113 1884 2626 -254 -510 - 288 MOTA 561 CB THR 72 -7.477 12.829 47.545 1.000 15.98 ANISOU 561 72 1700 CB THR 1761 2611 211 -458 - 421 ATOM 562 OG1 THR 72 -8.027 14.094 47.128 1.000 17.28 ANISOU 562 OG1 THR CG2 THR 72 2146 1553 2868 27 - 355 - 271 ATOM 72 -8.348 11.764 46.929 1.000 12.63 563 72 1296 1581 1923 -46 328 -1 72 -6.418 13.805 49.549 1.000 17.83 72 2153 1773 2847 -155 -1228 172 -5.216 13.536 49.329 1.000 20.17 72 2142 2265 3257 -225 -1049 CG2 THR ANISOU 563 328 - 127 ATOM 564 THR ANISOU 564 C THR -155 -1228 2 3 2 ATOM 565 0 THR ANISOU 565 O THR 72 2142 2265 3257 -225 -1049 480 2265 3257 -225 -1049 14.920 50.169 1.000 19.43 566 N ATOM 73 MET -6.785 ANISOU 566 N 73 2052 2455 -782 -451 -1 15.944 50.521 1.000 18.75 MET 2876 -782 -451 - 144 ATOM 567 CA MET 73 -5.799 ANISOU 567 CA MET 73 2117 2326 2682 -538 -466 - 280 15.338 51.480 1.000 22.03 MOTA 568 CB MET 73 -4.758 ANISOU 568 73 CВ MET 1826 2825 3/10 -3/7 -306 5 15.059 52.843 1.000 27.01 2853 3864 -04 3718 -377 -306 5 9 5 MOTA 569 CG 73 MET -5.374 ANISOU 569 CG MET 73 3545 -84 -87 1526 MOTA 570 SD 73 -4.107 14.850 54.107 1.000 32.23 MET ANISOU 570 SD MET 73 4364 4245 3637 469 -400 5 8 3 MOTA 571 CE 13.492 53.374 1.000 26.74 73 -3.179 MET ANISOU 571 CE MET 73 2885 4895 2381 326 425 1348 ATOM 572 C 73 -5.066 16.582 49.355 1.000 17.20 MET ANISOU 572 C MET 73 1338 2129 3067 -20 -269 -175ATOM 573 0 MET 73 -3.945 17.110 49.498 1.000 21.20 ANISOU 573 O MET ATOM 574 N ARG 73 1713 2512 3832 -541 51 -1024 74 -5.630 16.600 48.175 1.000 18.64 ANISOU 574 N ARG 74 1881 2051 3150 84 - 461 543 ATOM 575 CA ARG 74 -5.091 17.180 46.967 1.000 15.73 ANISOU 575 CAARG 74 937 1986 3053 169 27 - 174 576 ATOM СВ ARG 74 -5.655 16.537 45.704 1.000 16.53 ANISOU 576 СВ ARG 74 1711 1434 3137 -263 142 -160 577 ATOM CG ARG 74 -4.91116.934 44.440 1.000 15.01 ANISOU 577 CGARG 74 1270 1288 3144 -156 279 -554 MOTA 578 CD ARG 74 -5.683 16.543 43.185 1.000 16.10 ANISOU 578 CD ARG 74 1967 1031 3120 268 -92 -407 ATOM 579 ΝE ARG 74 -4.902 16.816 41.966 1.000 18.81 ANISOU 579 ΝE ARG 74 2259 1813 3075

-5.033 17.824 41.130 1.000 16.64

580

CZ

ARG

74

ATOM

-432 -252 -296

- 109 -CZ ARG 74 1968 ANISOU 580 1646 2709 -141 -190 - 596 NH1 ARG 74 -5.951 18.775 41.293 1.000 20.09 MOTA 581 ANISOU 581 NH1 ARG 74 1899 2075 3660 54 - 353 - 788 582 NH2 ARG 74 -4.220 17.896 40.068 1.000 20.12 ANISOU 582 NH2 ARG 74 2366 2844 2437 153 -196 - 400 ATOM 583 С ARG 74 -5.373 18.681 46.966 1.000 12.70 ANISOU 583 C 74 1187 ARG 1880 1758 6 -22 -136 ATOM 584 0 ARG 74 -4.501 19.465 46.582 1.000 14.07 ANISOU 584 0 ARG 74 1049 2048 2247 -221 -170 - 480 ATOM 585 Ν ARG 75 -6.567 19.099 47.387 1.000 12.72 ANISOU 585 N ARG 75 1402 1702 1.728 95 182 - 108 CA ARG ATOM 586 75 -7.006 20.471 47.308 1.000 13.40 CAANISOU 586 ARG 75 1924 1618 1548 87 275 - 193 587 СВ ATOM 75 ARG -7.737 20.784 45.995 1.000 13.45 ANISOU 587 CВ ARG 75 1972 1387 1751 -179 51 - 9ATOM 588 CGARG 75 -6.908 20.637 44.721 1.000 13.38 ANISOU 588 CG ARG 75 1638 1851 1594 78 -217 101 ATOM 589 CD ARG 75 -5.849 21.708 44.582 1.000 12.85 ANISOU 589 CDARG 75 1537 1602 1741 237 62 - 15 590 NE ARG ATOM 75 -5.087 21.685 43.347 1.000 13.71 ANISOU 590 ΝE ARG 75 1708 1797 1705 188 90 - 91 MOTA 591 CZARG 75 21.036 43.013 1.000 12.46 -3.984 ANISOU 591 1731 CZARG 75 1348 1656 -89 86 1 1 7 592 ATOM NH1 ARG 75 -3.418 20.241 43.894 1.000 14.64 ANISOU 592 NH1 ARG 75 1933 1794 1834 186 -91 6 5 ATOM 593 NH2 ARG 75 -3.444 21.167 41.794 1.000 13.72 ANISOU 593 NH2 ARG 75 1510 2037 1667 -136 84 - 83 ATOM 594 С ARG 75 -7.948 20.787 48.475 1.000 12.74 ANISOU 594 С ARG 75 1400 1656 1784 -209 214 -464ATOM 595 0 ARG 75 -8.780 19.944 48.818 1.000 14.60 ANISOU 595 Ω ARG 75 1348 1926 2273 -427 156 - 480 ATOM 596 N GLY 76 -7.830 21.955 49.078 1.000 11.92 ANISOU 596 N GLY 76 1537 1268 1724 -22 34 - 389ATOM 597 CA GLY 76 -8.801 22.395 50.070 1.000 12.44 ANISOU 597 CA $\operatorname{\mathsf{GLY}}$ 76 1439 1493 1796 -315 263 -412 ATOM 598 С GLY 76 -8.536 21.857 51.469 1.000 12.50 ANISOU 598 C GLY 76 1324 1900 5 326 - 273 1527 ATOM 599 0 GLY 76 -7.388 21.517 51.769 1.000 14.25 ANISOU 599 0 GLY 76 1100 2099 2218 -277 239 -225 N ATOM 600 PHE 77 -9.574 21.840 52.287 1.000 12.65 ANISOU 600 N PHE 77 1191 1806 1809 -162 231 -351 MOTA PHE 601 CA77 -9.526 21.474 53.694 1.000 14.00 ANISOU 601 PHE CA77 2110 1295 1914 -260 276 -138 PHE ATOM 602 CВ 77 -10.644 22.226 54.451 1.000 14.73 PHE ANISOU 602 СB 77 1554 2169 1874 -402 485 -317 603 CG PHE 77 -10.773 21.824 55.912 1.000 17.13 CG PHE ANISOU 603 77 2730 1849 -374 378 -243 22.369 56.886 1.000 19.49 1927 MOTA 604 CD1 PHE 77 -9.949 2744 ANISOU 604 CD1 PHE 77 2744 2700 1962 -119 219 -789 -11.730 20.902 56.309 1.000 19.13 605 ATOM CD2 PHE 77 ANISOU 605 CD2 PHE 77 2348 3068 1852 -501 864 -165 -10.068 21.973 58.217 1.000 19.75 2348 ATOM 606 CE1 PHE 77 ANISOU 606 CE1 PHE 77 2956 2956 2381 2168 -174 -313 - 1 -11.829 20.479 57.627 1.000 18.73 -174 -313 - 304 MOTA 607 CE2 PHE 77 ANISOU 607 CE2 PHE 77 2565 2711 1841 -382 310 - 77 -10.986 21.013 58.584 1.000 19.22 MOTA 608 CZ PHE 77. ANISOU 608 CZ77 PHE 2378 2542 2382 98 13 - 364 -9.668 19.976 53.924 1.000 13.73 MOTA 609 С 77 PHE ANISOU 609 C PHE 77 1306 2096 1813 -368 21 - 204 -10.520 19.313 53.291 1.000 16.02 ATOM 610 0 PHE 77 ANISOU 610 0 PHE 77 1386 2508 2194 -470 -128 - 425

- 110 -ATOM 611 N THR 78 -8.869 19.439 54.852 1.000 14.33 ANISOU 611 N THR 78 1543 2270 -472 35 - 49 1629 ATOM 612 CATHR 78 -9.034 18.053 55.276 1.000 15.80 ANISOU 612 CA THR 78 1813 2310 1880 -508 -23 8 2 MOTA 613 CB THR 78 17.081 54.666 1.000 18.26 -8.001 ANISOU 613 CB THR 78 1583 2199 3158 -599 334 131 614 OG1 THR MOTA 78 -7.92417.323 53.266 1.000 21.81 ANISOU 614 OG1 THR 78 3351 1877 3057 -88 943 - 370 ATOM 615 CG2 THR 78 -8.419 15.634 54.888 1.000 20.35 ANISOU 615 CG2 THR 78 2855 2254 2622 -1119 1108 - 707 616 ATOM C THR 17.881 56.777 1.000 19.14 78 -8.832 ANISOU 616 C THR 78 2845 2479 1948 -1747 -471 1 6 9 ATOM 617 THR 0 78 -7.801 18.311 57.290 1.000 22.04 ANISOU 617 0 THR 78 2781 2889 2704 -1718 -985 7 6 3 MOTA 618 N GLY 79 -9.730 17.203 57.484 1.000 19.20 ANISOU 618 79 N GLY 2629 2823 1844 -1352 19 4 5 ATOM 619 C.\ GLY 79 -9.429 16.695 58.819 1.000 16.69 ANISOU 619 CA GLY 79 1800 2770 1771 -518 196 - 95 ATOM 620 C GLY 79 -8.672 15.376 58.720 1.000 22.98 ANISOU 620 С GLY 79 2381 2874 3477 -272 -289 -545ATOM 621 0 GLY 79 -9.227 14.504 58.044 1.000 25.57 ANISOU 621 0 GLY 3683 79 2520 . 3514 -456 -974 - 141 ATOM 622 LEU 15.236 59.319 1.000 22.91 И 80 -7.494 ANISOU 622 2900 3392 30 - 206 - 60 14.081 59.072 1.000 25.08 Ν LEU 8 0 2412 30 - 206 - 606 ATOM 623 CA LEU 80 -6.644 ANISOU 623 CA LEU 2777 3904 206 621 361 13.294 60.370 1.000 24.30 80 2848 ATOM 624 С LEU 80 -6.372 ANISOU 624 С 80 2834 80 -5.729 LEU 2762 3637 -300 480 200 13.812 61.291 1.000 25.14 ATOM 625 0 LEU ANISOU 625 0 LEU 80 2253 3017 4283 27 145 - 5 14.480 58.415 1.000 27.16 CB LEU ATOM 626 80 -5.318 ANISOU 626 CB LEU 80 3057 3326 3937 379 918 641 MOTA 627 13.338 57.933 1.000 29.43 CG LEU 80 -4.411 ANISOU 627 СG LEU 80 3474 3505 4204 287 1260 1 7 3 628 ATOM CD1 LEU 12.438 56.956 1.000 38.31 80 -5.145 ANISOU 628 CD1 LEU 80 5673 3891 -1554 1987 - 287 4993 MOTA 629 CD2 LEU 80 -3.137 13.884 57.306 1.000 29.85 ANISOU 629 CD2 LEU 80 3502 3919 3920 125 1307 - 264ATOM 630 GLU 81 N -6*.*853 12.055 60.396 1.000 25.58 ANISOU 630 N GLU 81 2469 2759 4490 -196 -82 510 ATOM 631 CA GLU 81 -6.739 11.038 61.415 1.000 25.98 ANISOU 631 CA GLU 81 2739 2692 4441 -258 -55 424 ATOM 632 C GLU 81 -5.299 10.536 61.562 1.000 26.28 ANISOU 632 C GLU 81 2870 3268 3848 187 407 841 MOTA 633 0 GLU 81 -4.489 10.655 60.655 1.000 28.19 ANISOU 633 0 GLU 81 3709 3520 3483 253 799 - 544 CB GLU ATOM 634 81 -7.685 9.861 61.123 1.000 29.83 ANISOU 634 3533 CВ GLU 81 2894 4906 -770 270 181 MOTA 635 CG GLU 81 -7.241 8.832 60.098 1.000 25.34 ANISOU 635 CG GLU 81 1737 2915 4976 284 -1220 158 ATOM 636 CDGLU 81 -7.568 9.156 58.649 1.000 27.00 ANISOU 636 CD GLU 81 1841 3405 5012 475 -1887 - 456 ATOM 637 OE1 GLU 81 -8.120 10.240 58.324 1.000 28.81 ANISOU 637 OE1 GLU 81 3444 3091 4413 322 -155 7 9 1 ATOM 638 OE2 GLU 81 -7.240 8.273 57.814 1.000 31.31 ANISOU 638 OE2 GLU 81 3514 3384 4999 162 352 100 ATOM 639 M SER 82 -4.988 9.974 62.720 1.000 31.00 ANISOU 639 N SER 82 3568 3780 -65 4430 -30 1484 ATOM 640 CASER 82 -3.653 9.422 62.959 1.000 30.29 ANISOU 640 CASER 82 3692 3278 4540 -157 -515 1011 ATOM 641 SER 82 -3.421 8.150 62.150 1.000 31.76

- 111 -ANISOU 641 SER 82 C 3995 3241 4831 -102 -1104 8 4 7 642 ATOM 0 SER 82 61.397 1.000 34.01 -4.313 7.728 ANISOU 642 O SER 82 3193 3794 5935 458 -1188 1 3 4 643 ATOM CВ SER 82 -3.463 9.167 64.452 1.000 34.74 ANISOU 643 CB SER 4687 82 3907 4606 -232 -979 9 7 1 MOTA 644 OG SER 82 -2.36064.681 1.000 41.53 8.305 ANISOU 644 OG SER 82 4922 5366 5490 236 -1958 970 MOTA 645 GLY Ν 91 -17.230 9.498 70.136 1.000 42.64 ANISOU 645 M GLY 91 4516 7599 4086 -2166 2340 - 427 ATOM 646 CAGLY 91 -17.485 10.892 69.789 1.000 44.91 ANISOU 646 CAGLY 91 6666 7702 2697 -4311 -1561 5 6 5 ATOM 647 С GLY 91 -16.227 11.662 69.452 1.000 38.67 ANISOU 647 C 91 GLY 5455 1652 7587 -2821 -274 - 159 ATOM 648 0 GLY 91 -15.164 11.480 70.040 1.000 32.45 ANISOU 648 0 GLY 91 4241 4474 3616 -183 1152 - 439 MOTA 649 Ν GLY -16.332 12.558 68.474 1.000 31.97 92 ANISOU 649 N GLY 92 3881 5904 2363 -1382 735 - 571 650 ATOM CA-15.232 13.412 68.075 1.000 33.02 GLY 92 ANISOU 650 CAGLY 92 4121 6150 2274 -1716851 - 956ATOM 651 C GLY 92 -15.223 13.696 66.572 1.000 26.22 ANISOU 651 C GLY 92 2603 5046 2314 -885 741 -947MOTA 652 0 GLY 92 -16.289 13.666 65.939 1.000 23.91 ANISOU 652 0 GLY 92 2490 3396 3198 -680 548 -567 MOTA 653 M SER 93 -14.010 13.956 66.088 1.000 23.77 ANISOU 653 N SER 93 2405 3917 2708 -372 736 - 560 MOTA 654 CASER 93 -13.801 14.287 54.690 1.000 23.41 ANISOU 654 CASER 93 2700 3292 2901 -386 970 -399 ATOM 655 SER 93 -12.410 13.852 64.240 1.000 24.26 ANISOU 655 C SER 93 2547 3908 2763 -286 833 -224 MOTA 656 0 SER 93 -11.497 13.831 65.089 1.000 27.06 ANISOU 656 0 SER 93 3401 3536 3346 630 92 - 386 ATOM 657 CB SER 93 -13.966 15.795 64.467 1.000 25.71 ANISOU 657 CВ SER 93 2811 3225 3735 -576 271 - 506 ATOM 658 OG SER 93 -13.558 16.158 63.150 1.000 28.14 ANISOU 658 OG SER 93 2694 3713 4284 -373 290 MOTA 659 N TYR 94 -12.254 13.533 62.949 1.000 24.24 ANISOU 659 N TYR 94 2786 3320 3104 -204 791 -817 ATOM 660 94 CATYR -10.878 13.262 62.498 1.000 23.94 ANISOU 660 CATYR 94 3089 2502 3505 95 1112 - 683 ATOM 661 C TYR 94 -10.017 14.531 62.584 1.000 25.19 ANISOU 661 C TYR 94 2601 2657 4312 147 737 - 625 ATOM 662 0 TYR 94 -8.786 14.421 62.694 1.000 30.11 ANISOU 662 0 TYR 94 2617 3095 5726 307 760 3 6 MOTA 663 CB TYR 94 -10.800 12.659 61.098 1.000 25.64 ANISOU 663 CB TYR 94 3566 2910 3267 -293 1331 - 525 ATOM 664 CG TYR 94 -11.600 11.410 60.876 1.000 23.22 ANISOU 664 CG TYR 94 3359 2768 2697 -69 784 - 274 ATOM 665 CD1 TYR 94 -12.451 11.455 59.777 1.000 26.01 ANISOU 665 CD1 TYR 94 4410 2730 2741 499 353 - 543 MOTA CD2 TYR 666 -11.564 10.252 61.635 1.000 24.42 94 ANISOU 666 CD2 TYR 94 3117 2866 3297 73 458 - 1 4 CE1 TYR ATOM 667 94 -13.243 10.407 59.443 1.000 28.75 ANISOU 667 CE1 TYR 94 4559 3328 3037 434 140 - 1370 ATOM 668 CE2 TYR 94 -12.375 9.159 61.305 1.000 26.47 CE2 TYR ANISOU 668 94 4707 2585 2764 -220 1227 - 718 ATOM 669 CZTYR 94 -13.209 9.247 60.212 1.000 29.70 ANISOU 669 CZTYR 94 5641 3518 2125 -1172 1103 - 1447 ATOM 670 TYR OH 94 -14.059 8.281 59.730 1.000 34.02 ANISOU 670 TYR OH 94 3079 3962 5886 -423 1593 - 2638 ATOM 671 N SER 95 -10.628 15.714 62.561 1.000 22.61 ANISOU 671 \mathbf{N} SER 95 2460 2497 3632 -54 59 - 338

- 112 -CA SER 95 -9.924 16.975 62.750 1.000 22.54 672 ATOM ANISOU 672 CA SER 95 2257 2603 3706 -120 -301 4 6 673 С SER 95 -9.370 17.106 64.163 1.000 23.58 ANISOU 673 С SER 95 1811 3478 3671 -521 -88 -85 ATOM 674 O SER 95 -8.623 18.034 64.481 1.000 26.53 ANISOU 674 0 SER 95 2592 3242 4247 -469 -167 -641 675 CЗ ATOM SER 95 -10.838 18.177 62.478 1.000 27.58 ANISOU 675 СB SER 3657 2556 4264 365 -379 2 -11.506 18.093 61.242 1.000 39.40 95 3657 -379 2 8 MOTA 676 OG SER 95 ANISOU 676 OG SER 95 6336 4214 4421 900 -1445 1442 677 ATOM N ASP 96 16.194 65.060 1.000 25.04 -9.712 ANISOU 677 N ASP 96 2579 3688 3248 -399 277 - 232678 -9.228 16.317 66.422 1.000 24.42 ATOM CA ASP 96 ANISOU 678 CA ASP ANISOU 6/8 CA ASP ATOM 679 C ASP ANISOU 679 C ASP ATOM 680 O ASP ANISOU 680 O ASP ATOM 681 CB ASP ANISOU 681 CB ASP ANISOU 682 CG ASP ANISOU 682 CG ASP ATOM 683 OD1 ASP 96 2603 3347 3330 -470 257 -526 -7.735 16.050 66.501 1.000 24.45 96 96 2597 3228 3466 -471 162 -383 -7.073 16.589 67.404 1.000 26.51 96 96 2656 4047 3370 -170 160 -798 96 -9.952 15.334 67.334 1.000 24.97 96 2310 3806 3371 -423 -228 7 7 96 -11.411 15.605 67.606 1.000 26.77 96 2272 4334 3566 -362 -240 7 1 6 96 -11.935 16.723 67.388 1.000 33.94 96 3267 4894 4733 647 204 5 6 9 96 -12.058 14.646 68.083 1.000 32.65 ANISOU 683 OD1 ASP 684 OD2 ASP 3624 ANISOU 684 OD2 ASP 96 4709 4072 -1032 1446 - 202 -7.254 15.226 65.581 1.000 22.21 ATOM 685 N TYR 97 ANISOU 685 N 97 2292 3389 2760 -376 -77 -3 97 -5.835 14.852 65.583 1.000 23.71 TYR 2760 -376 -77 -102 686 CA TYR ATOM ANISOU 686 CA TYR 2480 3542 2987 -27 106 644 -5.026 15.828 64.743 1.000 23.06 97 ATOM 687 C 97 TYRANISOU 687 C TYR 2363 3754 2647 -410 -78 350 -3.992 16.327 65.230 1.000 24.29 97 ATOM 688 O TYR 97 ANISOU 688 O TYR 97 2205 3845 3178 -133 -230 7 4 -5.585 13.451 65.035 1.000 28.38 689 CB TYR ATOM 97 3230 3324 4229 540 -4508 -4.132 13.025 65.082 1.000 30.37 ANISOU 689 CB TYR 97 540 -450 8 3 2 ATOM 690 CG TYR 97 ANISOU 690 CG TYR 97 3278 766 -191 6 7 1 97 -3.511 12.691 66.285 1.000 30.19 CD1 TYR MOTA 691 ANISOU 691 CD1 TYR 97 2878 4475 4119 1106 151 951 97 -3.370 12.945 63.922 1.000 29.79 692 ATOM CD2 TYR ANISOU 692 CD2 TYR 3317 4005 3997 53 -253 544 -2.178 12.294 66.324 1.000 32.77 97 3317 4005 ATOM 693 CE1 TYR 97 ANISOU 693 CE1 TYR 97 2554 4771 5126 574 -68 763 ATOM 694 CE2 TYR -2.043 12.553 63.955 1.000 32.68 97 ANISOU 694 CE2 TYR 97 3536 3793 5087 403 353 323 ATOM 695 CZTYR 97 -1.445 12.228 65.157 1.000 33.00 ANISOU 695 CZTYR 97 2633 4284 5622 1066 264 456 ATOM 696 ОН TYR 97 -0.121 11.845 65.156 1.000 42.66 ANISOU 696 ОН TYR 97 2572 5373 8264 1161 764 1277 ATOM 697 CВ SER 98 -3.465 16.575 62.134 1.000 23.20 ANISOU 697 CВ SER 98 2461 2766 3587 105 2 -544 ATOM 698 OG SER 98 -3.632 15.649 61.078 1.000 26.49 ANISOU 698 OG SER 98 3824 3059 3180 -154 238 -457 ATOM 699 C SER 98 -5.694 17.744 61.701 1.000 18.66 ANISOU 699 C SER 98 2301 2150 2637 -295 66 1 3 ATOM 700 0 SER 98 -6.768 17.212 61.413 1.000 20.88 ANISOU 700 O SER 98 3042 2245 2646 -945 -249 1 8 1 ATOM 701 N SER 98 -5.457 16.110 63.511 1.000 23.62 ANISOU 701 N SER 98 2816 3227 2931 -441 -395 6 0 5 702 CA SER 98 -4.748 17.143 62.741 1.000 21.31 ATOM

- 113 -CA SER 98 2430 ANISOU 702 2687 2982 133 153 294 703 N MET 99 -5.307 18.891 61.148 1.000 18.68 ANISOU 703 N MET 99 2392 2722 -978 -366 1 0 1 1984 ATOM 704 CA MET 99 -6.047 19.560 60.075 1.000 17.84 CA MET 99 ANISOU 704 2431 2620 1726 -945 -212 - 17CB MET 705 99 -6.819 20.779 60.585 1.000 19.71 ANISOU 705 CB MET 99 2348 2968 2173 -679 25 6 4 ATOM 706 CG MET 99 -8.052 20.392 61.374 1.000 23.68 ANISOU 706 CG MET 99 2360 3055 3582 -504 393 489 707 99 -9.031 ATOM SD MET 21.821 61.911 1.000 22.33 ANISOU 707 SD MET 99 2569 3383 2534 -522 170 -120 708 ATOM CE MET 99 -8.148 22.225 63.419 1.000 36.98 ANISOU 708 CE MET 99 6485 4165 3401 -225 -1904 -23709 С -5.070 19.954 58.973 1.000 17.19 ATOM MET 99 709 C 710 O ANISOU 709 MET 99 2269 2488 1776 -960 -194 - 201ATOM MET 99 -3.964 20.341 59.324 1.000 16.93 ANISOU 710 O MET 99 1932 2583 1919 -367 -208 - 241ATOM 711 N CYS 100 -5.486 19.864 57.715 1.000 20.00 ANISOU 711 N CYS 100.3178 2683 1739 -1753 -358 1 6 6 100 -4.645 20.181 56.554 1.000 16.64 ATOM 712 CA CYS ANISOU 712 CA CYS 100 2213 2294 -924 -563 4 6 8 1817 MOTA 713 CB 100 -4.291 18.893 55.813 1.000 17.74 CYS ANISOU 713 CB CYS 100 2161 2174 2407 560 -765 1053 ATOM 714 SG CYS ANISOU 714 SG CYS 100 -3.035 18.928 54.552 1.000 33.56 100 5244 3511 3997 414 1509 6 0 1 715 C MOTA CYS 100 -5.347 21.121 55.590 1.000 13.48 ANISOU 715 C CYS 100 1879 1415 1829 -68 240 - 91 716 0 ATOM CYS 100 -6.585 21.127 55.496 1.000 14.49 ANISOU 716 O 100 1880 1952 1673 -497 -57 1 4 101 -4.589 21.921 54.852 1.000 13.35 101 1721 1677 1673 -254 -78 4 9 CYS 717 N ATOM TYR ANISOU 717 N TYR 101 1721 1677 1673 -254 -78 4 9 101 -5.016 22.753 53.755 1.000 10.27 718 CA TYR ANISOU 718 CA TYR 101 926 1498 ATOM 719 CB TYR ANISOU 719 CB TYR 101 1626 101 1626 1513 2027 -48 322 -101 -5.498 25.025 52.863 1.000 17.31 2027 -48 322 -236 MOTA 720 CG TYR ANISOU 720 CG TYR 101 2373 1509 2694 -158 -103 1 101 -6.815 25.068 52.519 1.000 16.38 2694 -158 -103 1 9 3 ATOM 721 CD1 TYR ANISOU 721 101 2464 CD1 TYR 752 3006 190 -227 5 5 ATOM 722 101 -7.307 25.715 51.412 1.000 17.01 CE1 TYR ANISOU 722 CE1 TYR 101 2755 714 2993 -86 -416 122 ATOM 723 CD2 TYR 101 -4.616 25.679 52.012 1.000 19.51 ANISOU 723 CD2 TYR 101 3032 1533 2847 -1143 -594 4 7 5 ATOM 724 CE2 TYR 101 -5.065 26.321 50.872 1.000 20.96 ANISOU 724 CE2 TYR 101 2802 1949 3211 238 112 769 ANISOU 725 CZ TYR 101 3238 2291 3126 -1228 -919 6 ATOM 726 OH TYR 101 -6.875 26.986 49.442 1.000 23.10 ANISOU 726 OH TYR 101 3141 3112 2522 -1228 -919 6 2 4 -14 -129 4 2 9 ATOM 727 C TYR 101 -4.041 22.518 52.596 1.000 11.25 ANISOU 727 C TYR 101 1223 1398 1654 727 C TYR 728 O TYR 728 O TYR 729 N SER 729 N SER -323 103 -252 ATOM 101 -2.823 22.677 52.787 1.000 12.23 ANISOU 728 O 101 1114 1750 1784 -87 130 - 20 ATOM 102 -4.542 22.190 51.405 1.000 11.17 ANISOU 729 N SER 102 1355 1279 1611 -220 145 - 263CA SER ATOM 730 102 -3.752 21.802 50.235 1.000 10.46 ANISOU 730 102 1144 1263 1568 62 - 1 - 125731 ATOM CВ SER 102 -4.027 20.343 49.908 1.000 13.46 ANISOU 731 ÇВ SER 102 1668 1212 2234 324 105 - 301 732 ATOM OG SER 102 -3.723 19.487 51.025 1.000 16.42 ANISOU 732 OG SER 102 2291 1313 2637 -122 -43 9 6

- 114 -ATOM 733 C SER 102 -4.046 22.668 49.008 1.000 11.74 ANISOU 733 C SER 102 1346 1500 1614 18 -39 - 10 ATOM 734 O SER 102 -5.148 23.148 48.784 1.000 12.84 ANISOU 734 O SER 102 1480 1410 1988 90 - 66 2 4 9 735 ATOM N MET 103 -3.004 22.871 48.187 1.000 12.33 ANISOU 735 N MET 103 1554 1722 1409 -262 -10 -246 736 ATOM CA MET 103 -3.188 23.603 46.938 1.000 12.92 ANISOU 736 CA MET 103 1663 1681 1565 22 47 - 7 G MOTA 737 CВ MET 103 -3.215 25.122 47.179 1.000 17.51 ANISOU 737 CВ MET 103 2439 1634 2579 -363 812 - 44 738 103 -1.929 25.808 47.549 1.000 20.07 ATOM CG MET ANISOU 738 MET CG 103 2509 1470 3646 -538 688 376 739 103 -2.136 27.614 47.689 1.000 18.10 ATOM SD MET ANISOU 739 SD MET 103 2235 1665 2975 -3 -334 -352 740 CE 103 -2.365 28.068 45.991 1.000 18.09 MOTA MET ANISOU 740 CE MET 103 2319 1457 3098 -187 -718 -214 741 C ATOM 103 -2.152 23.221 45.892 1.000 12.57 MET ANISOU 741 C MET 103 1420 1837 1519 119 -53 238 103 -1.120 22.573 46.175 1.000 12.57 103 1094 1891 1792 -155 -165 2 1 104 -2.418 23.650 44.655 1.000 12.83 742 0 ATOM MET ANISOU 742 O MET -155 -165 2 7 6 ATOM 743 N ANISOU 743 N GLY104 1493 104 -1.533 $\operatorname{GL} Y$ 1958 1422 237 -124 - 3 4 23.459 43.513 1.000 12.65 744 CA GLY ATOM 744 CA GLY 104 1075 2188 1544 -93 -37 242
745 C GLY 104 -1.624 24.622 42.542 1.000 14.36
745 C GLY 104 1909 1985 1561 -265 -294 142
746 O GLY 104 -2.033 25.700 42.967 1.000 15.69
746 O GLY 104 1628 2273 2060 163 -197 2 1 3
747 N THR 105 -1.242 24.397 41.276 1.000 14.52
747 N THR 105 1829 2182 1504 -59 -375 3 1 9
748 CA THR 105 -1.218 25.452 40.279 1.000 15.27
748 CA THR 105 1977 2223 1603 -105 363 3 65 ANISOU 744 CA GLY ATOM 745 C GLY ANISOU 745 C GLY ATOM 746 O GLY 104 -2.033 ANISOU 746 O GLY 104 1628 ATOM ANISOU 747 N MOTA ANISOU 748 CA THR 105 1977 2223 1603 -105 -363 3 6 5 CB THR 105 -0.359 25.083 39.039 1.000 15.61 CB THR 105 1936 2122 1873 -37 -106 59 OG1 THR 105 -0.884 23.876 38.446 1.000 16.16 MOTA 749 ANISOU 749 1873 -37 -106 5 5 4 MOTA 750 23.876 38.446 1.000 16.16 ANISOU 750 105 1738 OG1 THR 2260. 2140 217 -285 1 5 1 751 ATOM CG2 THR 105 1.092 24.882 39.369 1.000 17.47 ANISOU 751 CG2 THR 105 1918 2871 1847 -293 -227 5 2 7 752 C ATOM 105 -2.603 25.828 39.755 1.000 14.73 THR ANISOU 752 C THR 105 1989 1694 1913 122 -340 1 9 9 753 O THR ATOM 105 -2.730 26.921 39.174 1.000 19.91 ANISOU 753 O THR 105 2579 2355 754 N ALA 106 -3.587 2632 23 -437 1004 ATOM 24.960 39.913 1.000 16.57 N ALA 106 1836 ANISOU 754 2413 2047 2 -260 661 ATOM 755 CA ALA 106 -4.975 25.167 39.465 1.000 14.94 CA ALA 106 1975 CB ALA 106 -5.054 ANISOU 755 1904 1798 105 -456 3 6 5 756 ATOM 24.945 37.965 1.000 17.75 ANISOU 756 CB ALA 106 2006 2862 1876 140 -201 -24.251 40.222 1.000 16.26 140 -201 - 3 2 ATOM 757 C ALA 106 -5.942 ANISOU 757 C ALA 106 1710 2174 2293 327 -127 4 9 1 758 O ALA 106 -5.498 ATOM 23.398 41.013 1.000 14.57 ANISOU 758 O ALA 1971 1945 213 -21 3 24 410 40 008 1 000 16 7 1 106 1622 213 -21 3 3 7 ATOM 759 N ASP 107 -7.253 ANISOU 759 N ASP 107 1768 2096 2485 540 -22 3 0 4 760 CA 23.638 40.633 1.000 16.10 ATOM 107 -8.310 ASP ANISOU 760 CA ASP 107 1696 2175 51 - 485 - 14 2246 ATOM 761 CB ASP 107 -8.231 22.171 40.211 1.000 17.09 ANISOU 761 CB ASP 107 1299 2385 2808 144 -203 - 399 ATOM 762 CG 107 -8.418 21.966 38.720 1.000 21.54 ASP ANISOU 762 CG ASP 107 2385 2894 2906 84 - 317 - 722 MOTA 763 OD1 ASP 107 -9.452 22.445 38.189 1.000 23.92

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ANISOU			ASP	107	3447	2970	2672	698 -753 - 772
ATOM	764		ASP		-7.563	21.311	38.080	1.000 24.88
ANISOU ATOM	765	C C	ASP	107		4004	2954	105 244 -679
ANISOU		C .	ASP ASP	107		23.785	42.160	1.000 14.16
ATOM	766	0	ASP	107 107		1918	2201	237 -447 1 5 3
ANISOU		ŏ	ASP	107		22.850 1927	42.936	1.000 16.67
ATOM	767	Ñ	ASN		-8.027	25.020	2390 42.598	-189 -193 9 7
ANISOU		N	ASN	108		1866	1870	1.000 15.34 82 51 2 3 9
ATOM	768	CA	ASN	108	-7.967	25.314	44.031	1.000 13.68
ANISOU		CA	ASN	108	1479	1823	1898	153 107 257
ATOM ANISOU	769 769	CB	ASN	108		26.420	44.272	1.000 15.60
AMISOU	770	CB CG	ASN ASN	108	1593	2026	2309	16 267 - 98
ANISOU	-	CG	ASN	108	-5.516 1505	25.942	43.963	1.000 15.23
ATOM	771		ASN	108	-5.086	2141 24.932	2142	5 -53 2
ANISOU			ASN		1412	24.332	44.505 1998	1.000 15.40
MOTA	772	ND2	ASN		-4.823	26.678	43.094	-5 -239
ANISOU	_		ASN	108	1593	2198	2652	339 393 222
ATOM	773	C	ASN		-9.310	25.708	44.642	1.000 14.55
ANISOU ATOM		C	ASN	108	1471	1937	2120	261 191 5 2 6
ANISOU	774 774	0	ASN	108	-10.222		43.958	1.000 16.89
ATOM	775	N	ASN LEU		1861 -9.412	2336	2219	716 -109 1 4
ANISOU		N	LEU	109		25.512 1648	45.954	1.000 13.42
ATOM	776	CA	LEU		-10.602	1048 25 796	1994 46.769	179 130 9
ANISOU		CA	LEU	109	1094	2122	1923	1.000 13.53 -52 -86 -256
ATOM	777	СB	LEU	109	-11.187	24.499	47.331	1.000 14.50
ANISOU		CB	LEU	109	1382	1959	2169	119 455 - 468
ATOM ANISOU	778 778	CG	LEU	109	-11.580		46.370	1.000 15.21
ATOM	779	CG CD1	LEU	109	1593	1785	2403	235 63 - 342
ANISOU	_		LEU	109	-11.931 2460	22.083 1674	47.089	1.000 18.26
ATOM	780	CD2			-12.780	10/4	2806 45.529	382 -414 - 9 4
	780	CD2		109	3055	2391	3052	1.000 22.36 44 -1155 288
ATOM	781	С	LEU		-10.203	26.794	47.840	1.000 13.54
ANISOU		C	LEU	109	1179	1989	1979	76 -116 - 259
ATOM ANISOU	782	0	LEU		-9.416	26.428	48.717	1.000 16.15
ATOM	783	N O	LEU PHE	109	2196	2210	1730	-52 -366 3 2
ANISOU		N	PHE	110	-10.706 1369		47.786	1.000 16.11
ATOM	784	CA	PHE		-10.298	2042	2709	105 -118 - 288
ANISOU	784	CA	PHE		1626	1801	48.732 3050	1.000 17.05 -116 259 - 362
ATOM	785	CB	PHE		-9.660	30.259	47.991	1.000 17.94
ANISOU		СВ	PHE	110	1423	2366	3027	-290 228 -129
ATOM ANISOU	786	CG	PHE		-8.425	29.972	47.165	1.000 20.32
ATOM	787	CG CD1	PHE		1702	2650	3368	-176 459 -385
ANISOU		CD1		110	-7.257 1885	29.598	47.793	1.000 20.35
ATOM	788	CD2			-8.405	2462 30.110	3387	461 573 - 707
ANISOU	788	CD2	PHE	110	2073	2226	45.789 3419	1.000 20.31 512 712 - 264
ATOM	789	CE1	PHE		-6.102	29.347	47.065	1.000 19.49
ANISOU		CE1	PHE	110	1958	2116	3332	176 749 -631
ATOM ANISOU	790	CE2			-7.288	29.846	45.050	1.000 20.65
ATOM	790 791	CE2	PHE		2158	2094	3596	758 724 - 321
ANISOU		CZ CZ	PHE PHE	110	-6.118	29.496	45.694	1.000 19.43
ATOM	792	C	PHE		1925 -11.495	2131	3327	219 542 - 780
ANISOU		C	PHE	110	1774	29.556 1806	49.538 2911	1.000 17.08
ATOM	793	Ō	PHE		-12.562	29.792	48.929	-74 414 -111 1.000 21.26
ANISOU	793	0	PHE	110	1849	2577	3650	405 178 - 448
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NATISOU 794 N	ATOM 794 N	PRO	111 -11.406	20 717	50.851	1.000 19.41
ATOM 795 CD PRO 111 -10.278 29.322 51.705 1.000 19.20 ANISOU 795 CD PRO 111 -12.731 1880 2640 -417 255 -514 ATOM 796 CA PRO 111 -12.549 30.252 51.604 1.000 21.47 255 -514 ATOM 796 CA PRO 111 3025 1924 30.252 51.604 1.000 21.47 ATOM 797 CB PRO 111 3025 1924 30.252 51.604 1.000 21.47 ATOM 797 CB PRO 111 3789 2054 31.77 314 776 -575 ATOM 798 CG PRO 111 -10.775 29.535 53.100 1.000 23.63 3 ATOM 798 CC PRO 111 -12.67 30.007 53.055 1.000 23.63 3 ATOM 798 CG PRO 111 -12.828 31.779 51.700 1.000 23.63 4 776 -575 ATOM 798 CG PRO 111 -12.828 31.779 51.700 1.000 23.63 8 ATOM 800 O PRO 111 3139 2049 3887 79 -142 -479 ATOM 800 O PRO 111 3139 22.194 51.834 1.000 25.79 7 ATOM 800 O PRO 111 3139 22.194 51.834 1.000 25.79 7 ATOM 801 N SER 112 -511.906 23.517 50.872 1.000 25.79 7 ATOM 801 N SER 112 -511.906 23.517 50.872 1.000 25.19 7 ATOM 802 CA SER 112 2654 2655 4734 496 1364 45 ATOM 803 CB SER 112 -12.506 31.919 50.631 1.000 26.73 7 ANISOU 803 CB SER 112 -12.506 31.919 50.631 1.000 26.73 7 ANISOU 804 OG SER 112 -111.322 3663 5855 172 2582 -510 ATOM 805 C SER 112 2613 2546 49.54 10.000 33.77 ANISOU 805 C SER 112 2613 2546 49.54 10.000 36.79 40.000 37.74 ANISOU 806 O SER 112 2613 2546 49.54 10.000 36.79 40.000 36.79 ANISOU 806 O SER 112 2613 2546 49.54 10.000 36.79 40.000 36.79 40.000 37.74 10.000 37.74 10.000 37.75 ANISOU 806 O SER 112 2613 2546 49.54 10.000 36.79 40.000 37.74 40.000 37.74 10.000 37.75 40.000 37.74 40.000 37.74 10.000 37.75 40.000 37.74 10.000 37.75 40.000 37.74 10.000 37.75 40.000 37.74 10.000 37.75 40.000 37.74 10.000 37.75 4						
ANISOU 795 CD PRO 111 2773 1880 2640 -417 255 -514 ATOM 796 CA PRO 111 3026 1924 30.252 51.604 1.000 21.47 7 ANISOU 797 CB PRO 111 3026 1924 32.66 -50 728 -655 ATOM 797 CB PRO 111 3789 2054 3137 33.055 1.000 23.68 ANISOU 797 CB PRO 111 3789 2054 3137 33.055 1.000 23.68 ANISOU 798 CG PRO 111 2767 2908 2809 -1006 623 -414 ANISOU 800 CPRO 111 3139 2049 3887 79 -142 -479 ANISOU 800 CPRO 111 3139 2049 3887 79 -142 -479 ANISOU 800 CPRO 111 3139 2049 3887 79 -142 -479 ANISOU 800 CPRO 111 3139 2049 3887 79 -142 -479 ANISOU 800 CPRO 111 3139 32.194 51.834 1.000 25.19 ANISOU 801 N SER 112 -11.906 32.517 50.872 1.000 25.19 ANISOU 801 N SER 112 3514 2269 3788 -447 -8552 82 ATOM 802 CA SER 112 -2654 0255 4734 496 1364 45 6 ATOM 803 CB SER 112 12654 0255 4734 496 1364 45 6 ATOM 804 OG SER 112 6530 2154 5351 1902 26.62 ANISOU 800 CPRO 111 3132 34.719 52.688 1.000 36.94 ANISOU 804 OG SER 112 6530 2154 5351 1902 26.62 ANISOU 806 CSER 112 2613 2546 4956 1021 16666 51 ATOM 806 CSER 112 2613 2546 4956 1021 16666 65 1 ATOM 808 CA GLY 113 3292 247 508 645 800 837 -400 ATOM 808 CA GLY 113 2992 36.06 102 881 798 1400 ATOM 809 C GLY 113 3292 247 508 645 800 837 -400 ATOM 808 CA GLY 113 2992 36.06 502 881 798 1400 ATOM 809 C GLY 113 3297 247 508 655 1000 22.81 ANISOU 800 CBLY 113 3297 247 508 655 1000 22.81 ANISOU 800 CBLY 113 3297 247 508 655 1000 30.79 SANISOU 801 CA GLY 113 2992 36.06 502 881 798 1400 ATOM 808 CA GLY 113 2992 36.06 502 887 795 28 ANISOU 801 CA GLY 113 3297 37.463 502 887 797 52.84 ANISOU 801 CA GLY 113 3297 366 502 36.94 300 80 CA GLY 113 3297 360 502 364 500 807 79 500 800 800 800 CA GLY 113 3297 319 486 65 1000 30.79 500 800 CA GLY 113 3297 319 486 65 1000 30.79 500 800 CA GLY 113 3297 319 486 65 1000 30.79 500 800 CA GLY 113 3297 319 486 65 1000 30.79 500 800 CA GLY 113 3297 319 486 65 1000 30.79 500 800 CA GLY 113 389 300 500 79 500 800 CA GLY 113 3297 320 500 500 79 500 800 CA GLY 113 3297 320 500 500 79 500 800 CA GLY 113 3297 320 500 500 79 500 800 CA GLY 113 3297 320 500 500 79 500 800 500 79 500 800 60 CA GL	ATOM 795 C	-				
ANISOU 796 CA PRO 111 3022 1924 3206 -50 728 -635 ATOM 797 CB PRO 111 -12.167 30.007 3.631 30.007 3.631 ANISOU 797 CB PRO 111 3789 2054 3137 334 776 -575 ATOM 798 CG PRO 111 -10.775 29.535 53.100 1.000 23.63 -414 ATOM 799 C PRO 111 -12.167 29.535 53.100 1.000 23.88 ANISOU 798 CG PRO 111 -12.167 29.535 53.100 1.000 23.88 ANISOU 798 CG PRO 111 -12.282 31.739 51.433 1.000 23.88 ANISOU 799 C PRO 111 -13.919 32.194 51.433 1.000 23.88 ANISOU 800 O PRO 111 -13.919 32.194 51.834 1.000 26.77 ANISOU 800 O PRO 111 -13.919 32.194 51.834 1.000 26.77 ANISOU 801 N SER 112 -11.906 32.517 50.872 1.000 25.19 ANISOU 801 N SER 112 -12.300 33.919 50.631 1.000 25.19 ANISOU 801 N SER 112 -12.506 34.712 51.834 1.000 26.43 ANISOU 802 CA SER 112 -12.506 34.712 51.912 1.000 25.19 ANISOU 803 CB SER 112 -12.506 34.712 51.912 1.000 25.19 ANISOU 803 CB SER 112 -12.506 34.712 51.912 1.000 33.37 ANISOU 804 CG SER 112 -12.506 34.712 51.912 1.000 33.37 ANISOU 805 C SER 112 -12.2614 255 474 4.96 1364 45.6 ANISOU 804 CG SER 112 -12.2614 255 474 4.96 1364 45.6 ANISOU 805 C SER 112 -12.2614 255 474 4.96 1364 45.6 ANISOU 806 C SER 112 -12.2614 2782 34.719 52.688 1.000 36.94 ANISOU 806 C SER 112 -12.12.261 32.546 49.56 10.21 1668 65 1 ANISOU 806 C SER 112 -12.12.261 34.587 49.723 1.000 26.6.25 1 ANISOU 806 C SER 112 2613 2546 49.56 10.21 1668 65 1 ANISOU 806 CA GLY 113 2937 2947 5108 10.00 22.5.85 1 ANISOU 808 CA GLY 113 2937 39.40 49.41 4.000 22.5.85 1 ANISOU 808 CA GLY 113 2932 36.478 84.365 1.000 30.79 81 4.000 22.81 80.00 837 -400 ANISOU 810 CA SEP 114 -8.257 37.463 51.122 1.000 25.85 1 ANISOU 810 CA SEP 114 -7.910 30.60 37.47 458 50.366 1.000 30.3 81 ANISOU 810 CA SEP 114 -7.910 30.60 37.47 458 50.366 1.000 25.85 1 ANISOU 810 CA SEP 114 -7.910 30.60 37.47 458 50.366 1.000 25.85 1 ANISOU 810 CA SEP 114 -7.910 30.60 37.47 458 50.366 1.000 25.85 1 ANISOU 810 CA SEP 114 -7.910 30.60 37.47 458 50.366 1.000 25.85 1 ANISOU 810 CA SEP 114 -7.910 30.20 30.40 40.77 7 ANISOU 810 CA SEP 114 -7.910 30.20 30.40 40.77 7 ANISOU 810 CA SEP 114 -7.910 30.20 30.40		D PRO	111 2773	1880	2640	-417 255 -514
ATOM 797 CB PRO 111 -12 167 30 007 53 055 1 000 23 63 63 ANISOU 797 CB PRO 111 3789 2054 3137 314 776 -5 75 ATOM 798 CG PRO 111 -10 775 29 535 53 100 1 000 22 .33 ANISOU 798 CF PRO 111 -12 .28 31.739 51 .433 1000 23 .88 ANISOU 799 C PRO 111 -12 .28 31.739 51 .433 1000 23 .88 ANISOU 800 O PRO 111 -13 .919 32 .194 51 .834 1 .000 26 .77 ANISOU 800 O PRO 111 3189 20 69 32 .517 50 .872 1 .000 25 .19 ANISOU 801 N SER 112 -11 .906 32 .517 50 .872 1 .000 25 .19 ANISOU 801 N SER 112 -11 .906 32 .517 50 .872 1 .000 25 .19 ANISOU 802 CA SER 112 26364 2655 4734 496 1364 45 6 ATOM 803 CB SER 112 -12 .250 30 33 .919 50 .631 1 .000 26 .43 ANISOU 803 CB SER 112 -12 .250 36 34 .712 51 .912 1 .000 25 .19 ANISOU 804 OG SER 112 -12 .250 36 34 .712 51 .912 1 .000 33 .3 7 ANISOU 805 C SER 112 2650 21 .44 5 .25						
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- 117 -ANISOU 824 CD2 PHE 115 1933 1931 2927 7 298 - 810 825 CE1 PHE 115 -7.100 29.711 54.163 1.000 20.25 ANISOU 825 CE1 PHE 115 2825 3042 1825 317 341 - 575 115 -6.338 29.412 51.955 1.000 19.11 ATOM 826 CE2 PHE ANISOU 826 CE2 PHE 115 1865 2158 3237 336 351 -885 MOTA 827 CZ PHE 115 -6.452 28.936 53.233 1.000 19.39 ANISOU 827 CZ PHE 115 2068 1910 3390 320 248 - 669 ATOM 828 С PHE 115 -6.506 33.624 50.327 1.000 17.86 ANISOU 828 С PHE 115 1964 1945 2878 61 344 1 6 ATOM 829 O ANISOU 829 O ATOM 830 N ANISOU 830 N ATOM 831 CA 115 -5.324 33.315 50.271 1.000 17.34 PHE PHE 115 1868 2107 2613 -132 179 157 GLU 116 -7.310 33.683 49.263 1.000 18.21 GLU 116 1921 1934 3065 547 281 6 2 831 CA GLU ATOM 116 -6.848 33.387 47.907 1.000 19.99 ANISOU 831 CA $\operatorname{\mathsf{GLU}}$ 116 2128 2618 2851 81 231 2 2 2 MOTA 832 CЗ GLU 116 -7.968 33.605 46.884 1.000 18.61 ANISOU 832 CВ GLU 116 2058 1952 3060 231 244 270 833 ATOM CG GLU 116 -7.398 33.378 45.482 1.000 18.61 ANISOU 833 CG GLU 116 1813 2288 2971 -32 - 33 295 ATOM 834 CDGLU 116 -8.442 33.230 44.412 1.000 22.40 ANISOU 834 CDGLU 116 1908 3193 3410 -122 -278 - 91 OE1 GLU ATOM 835 116 -9.654 33.272 44.678 1.000 30.82 ANISOU 835 OE1 GLU 116 1793 4465 5452 273 -414 - 24MOTA 836 OE2 GLU 116 -8.085 33.063 43.225 1.000 30.24 ANISOU 836 OE2 GLU 116 3333 5132 3026 382 -658 3 2 7 837 GLU 116 -5.620 34.211 47.535 1.000 18.82 ANISOU 837 GLU 116 2090 2069 2990 294 119 487 ATOM 838 0 GLU 116 -4.605 33.701 47.049 1.000 17.41 ANISOU 838 O GLU 116 2228 1780 2606 45 259 282 ATOM 839 117 -5.660 Ν ARG 35.508 47.777 1.000 21.02 ANISOU 839 N ARG 117 2313 2185 3487 408 220 9 0 ATOM 840 CA ARG 117 -4.560 36.420 47.431 1.000 21.35 ANISOU 840 CA ARG 117 2337 1800 3976 466 147 ATOM 841 C ARG 117 -3.291 36.054 48.192 1.000 20.52 ANISOU 841 C ARG 117 2292 2124 3380 353 288 - 10 ATOM 842 O ARG 117 -2.186 35.969 47.636 1.000 18.96 ANISOU 842 0 ARG 117 2223 1664 3316 318 231 138 ATOM 843 CB ARG 117 -4.971 37.885 47.693 1.000 25.59 ANISOU 843 CB ARG 117 3237 1900 4587 929 1882 6 3 2 ATOM 844 CG ARG 117 -3.881 38.908 47.478 1.000 32.57 ANISOU 844 CG ARG 117 5212 1925 5237 -281 1083 6 2 3 ATOM 845 CDARG 117 -4.325 40.323 47.859 1.000 36.56 ANISOU 845 CD ARG 117 6009 2157 5724 149 1774 6 6 3 ATOM 846 ΝE ARG 117 -5.162 40.335 49.056 1.000 44.43 ANISOU 846 117 7200 ΝE ARG 3742 5940 -96 2344 - 15MOTA 847 CZARG 117 -4.763 40.501 50.306 1.000 45.48 ANISOU 847 CZARG 117 6422 4804 6054 -370 2388 - 283 MOTA 848 NH1 ARG 117 -3.484 40.683 50.619 1.000 53.21 ANISOU 848 NH1 ARG 117 6867 6451 6900 -2543 2487 3 5 4 849 NH2 ARG 117 -5.647 40.487 51.301 1.000 50.00 ANISOU 849 NH2 ARG 117 6265 6511 6220 224 2433 - 1534 35.832 49.493 1.000 19.30 ATOM 850 N ILE 118 - 3.439ANISOU 850 N ILE 118 2275 1838 3221 128 407 - 645 35.527 50.331 1.000 18.25 MOTA 851 CAILE 118 -2.275 ANISOU 851 CAILE 118 2376 1745 2811 78 530 - 449 35.597 51.820 1.000 18.24 ATOM 852 CB ILE 118 -2.665 ANISOU 852 CB ILE 118 2201 1726 3003 346 906 - 306 34.851 52.732 1.000 18.49 3003 MOTA CG2 ILE 853 118 -1.712 ANISOU 853 CG2 ILE 118 2077 2158 2792 118 2077 2158 2792 -202 306 -118 -2.877 37.031 52.368 1.000 24.69 -202 308 -530 ATOM 854 CG1 ILE ANISOU 854 CG1 ILE 118 4436 1808 3136 284 1382 - 414

- 118 -855 CD1 ILE 118 -3.786 37.025 53.582 1.000 29.63 ATOM ANISOU 855 CD1 ILE 118 6169 3096 1258 - 1068 1994 189 MOTA 856 C ILE 118 -1.692 49.959 1.000 15.65 34.172 ANISOU 855 C ILE 118 2316 1549 2082 -89 573 - 117 857 ILE 118 -0.463 MOTA 34.035 49.802 1.000 14.59 ANISOU 857 0 ILE 118 2240 1255 2051 16 286 214 858 N TRP 119 - 2.52333.139 49.784 1.000 14.44 ATOM ANISOU 858 NTRP 119 2125 1592 1771 47 128 - 71 CA859 TRP MOTA 119 -2.010 31.795 49.518 1.000 13.68 ANISOU 859 C.A. TRP 119 1712 1529 1957 -61 220 4 0 860 CЗ TRP 119 -3.089 30.755 49.932 1.000 14.93 MOTA ANISOU 860 CВ TRP 119 1819 1729 2123 -234 295 **-**35 119 -2.864 861 CG TRP ATOM 30.482 51.420 1.000 16.19 ANISOU 861 CG TRP 119 1640 2364 2146 -168 582 167 CD2 TRP MOTA 862 119 -2.116 29.430 51.993 1.000 20.41 ANISOU 862 CD2 TRP 119 3189 2414 2151 202 523 405 863 CE2 TRP 119 -2.177 ATOM 29.580 53.392 1.000 19.84 ANISOU 863 CE2 TRP 119 3536 1818 2184 -439 234 137 CE3 TRP ATOM 864 119 -1.390 28.357 51.456 1.000 23.94 ANISOU 864 CE3 TRP 119 5382 1647 2068 561 126 400 CD1 TRP ATOM 865 119 - 3.34031.223 52.460 1.000 20.05 CD1 TRP ANISOU 865 119 3207 -9 189 -139 2343 2069 866 NE1 TRP ATOM 119 -2.938 30.689 53.649 1.000 20.32 ANISOU 866 NE1 TRP 119 2806 2726 -96 2188 -68 -185 CZ2 TRP ATOM 867 119 -1.547 28.714 54.281 1.000 22.12 ANISOU 867 CZ2 TRP 119 4071 2256 -17 105 2 2 2078 868 CZ3 TRP 119 -0.761 ATOM 27.490 52.332 1.000 21.52 ANISOU 868 CZ3 TRP 119 4214 2168 1794 311 -193 1 9 7 869 CH2 TRP ATOM 119 - 0.84727.674 53.715 1.000 24.34 ANISOU 869 CH2 TRP 119 5349 2047 1850 329 148 183 870 TRP 119 -1.521 48.095 1.000 14.27 ATOM С 31.634 ANISOU 870 С TRP 119 2180 1259 -187 334 - 65 1985 ATOM 871 0 TRP 119 -0.569 30.865 47.855 1.000 14.73 ANISOU 871 0 TRP 119 1996 1653 1946 -67 362 101 ATOM 872 N THR 120 -2.109 32.325 47.116 1.000 13.99 ANISOU 872 Ν THR 120 2231 1237 1848 106 627 -137 ATOM 873 CATHR 120 -1.541 32.275 45.762 1.000 15.19 ANISOU 873 CATHR 120 1903 2093 9 435 - 242 1774 874 CB ATOM THR 120 - 2.49232.983 44.787 1.000 16.41 ANISOU 874 1995 -331 152 6 6 44.766 1.000 18.53 CВ THR 120 1934 2304 875 OG1 THR MOTA 120 -3.738 32.297 ANISOU 875 OG1 THR 120 1891 -236 195 407 2288 2863 MOTA 876 CG2 THR 120 -1.974 32.906 43.358 1.000 18.02 CG2 THR ANISOU 876 120 2135 2602 2108 324 322 3 1 8 THR 32.870 45.727 1.000 14.19 ATOM 877 С 120 -0.145 ANISOU 877 С THR 120 1868 87 285 -167 2050 1475 MOTA 878 32.299 45.078 1.000 13.62 0 THR 120 0.756 ANISOU 878 0 THR 120 1864 1692 1620 301 354 217 MOTA 879 GLN 121 0.114 33.962 46.429 1.000 14.55 ANISOU 879 1672 N GLN 121 1721 175 - 67 2136 304 ATOM 880 CA 121 1.459 GLN 34.548 46.483 1.000 15.80 ANISOU 880 CA GLN 121 2067 1666 -18 -119 3 6 2 .2271 ATOM 881 С GLN 121 2.465 33.642 47.176 1.000 13.73 C ANISOU 881 GLN 121 1747 1665 1806 -30 18 1 1 4 MOTA 882 Q GLN 121 3.603 33.452 46.685 1.000 15.36 ANISOU 882 0 GLN 121 2063 1688 2084 48 360 - 44 MOTA 883 CB GLN 121 1.315 47.154 1.000 18.85 35.918 ANISOU 883 121 2537 CВ GLN 1426 3200 -73 -5356 MOTA 884 CG GLN121 2.639 36.558 47.543 1.000 18.88 ANISOU 884 GLN CG 121 2507 1788 59 9 - 248 2878 ATOM 885 CD GLN 121 3.468 36.936 46.337 1.000 20.70

- 119 -ANISOU 885 CD GLN 121 2584 2138 -373 -85 231 3142 OE1 GLN 121 2.935 886 37.088 45.224 1.000 22.47 ANISOU 886 OE1 GLN 121 2695 2822 3019 -245 0 121 887 NE2 GLN 37.101 46.522 1.000 25.22 121 4.779 ANISOU 887 NE2 GLN 121 2426 3344 3811 127 -131 1 3 8 5 ATOM 888 N 122 2.081 TYR 33.054 48.299 1.000 12.26 ANISOU 888 N TYR122 1747 1514 1399 99 - 55 - 258 889 CA TYR 122 2.896 ATOM 32.102 49.050 1.000 13.18 ANISOU 889 CA TYR 122 1901 1643 1464 -20 -253 - 160 890 CB TYR 122 2.211 ATOM 31.724 50.364 1.000 13.78 ANISOU 890 CB TYR 122 2045 1435 116 48 - 28 1756 891 ATOM CG TYR 122 2.994 30.808 51.282 1.000 14.22 ANISOU 891 CG TYR 122 1966 1681 1758 68 1 0 1 101 892 CD1 TYR 122 4.271 ATOM 31.120 51.722 1.000 17.48 ANISOU 892 CD1 TYR 122 1788 1972 2882 149 -5 4 2 0 893 CE1 TYR 122 5.003 ATOM 30.284 52.576 1.000 18.55 ANISOU 893 CE1 TYR 122 2131 2050 2868 102 -404 2 5 1 ATOM 894 CD2 TYR 122 2.445 29.619 51.731 1.000 20.72 ANISOU 894 CD2 TYR 122 3308 1366 3197 -519 -1524 3 2 3 ATOM 895 CE2 TYR 122 3.140 28.773 52.574 1.000 25.40 ANISOU 895 CE2 TYR 122 3772 1812 4067 -782 -2084 873 ATOM 896 CZTYR 122 4.413 29.101 52.992 1.000 20.93 ANISOU 896 CZTYR 122 2985 1742 3224 -96 -1145 3 1 3 ATOM 897 ОН TYR 122 5.068 28.230 53.826 1.000 29.87 ANISOU 897 OH TYR 122 4830 1998 4522 -680 -3078 621 898 ATOM С TYR 122 3.218 30.876 48.209 1.000 12.33 ANISOU 898 C TYR 122 1833 1412 1439 89 -218 8 8 ATOM 899 O 122 4.395 122 1896 TYR 30.507 48.117 1.000 14.25 ANISOU 899 O TYR 1861 1656 339 -242 2 1 6 900 N ATOM PHE 123 2.224 30.269 47.573 1.000 11.28 ANISOU 900 N PHE 123 1950 1297 1041 6 -151 185 MOTA 901 CA PHE 123 2.482 29.151 46.665 1.000 12.08 ANISOU 901 CA PHE 123 1731 1219 1640 64 - 60 2 6 ATOM 902 CB PHE 123 1.139 28.719 46.024 1.000 13.86 ANISOU 902 CB PHE 123 2048 1550 1666 -104 -276 - 82 903 ATOM CG PHE 123 1.311 27.516 45.099 1.000 14.44 ANISOU 903 CG PHE 123 2173 1677 1637 142 -475 - 94ATOM 904 CD1 PHE 123 1.281 26.234 45.614 1.000 13.64 ANISOU 904 CD1 PHE 123 1857 1563 1764 -42 -702 - 236ATOM 905 CD2 PHE 123 1.511 27.664 43.729 1.000 13.81 ANISOU 905 CD2 PHE 123 1450 2164 1634 -420 -295 - 248 ATOM 906 CE1 PHE 123 1.468 25.141 44.795 1.000 17.16 ANISOU 906 CE1 PHE 1819 123 2282 2418 130 -855 - 644 MOTA 907 CE2 PHE 123 1.715 26.559 42.916 1.000 18.31 ANISOU 907 CE2 PHE 123 2098 2657 -1053 172 -845 2201 MOTA 908 CZ PHE 123 1.706 25.295 43.445 1.000 16.71 ANISOU 908 CZ PHE 123 1442 2382 2526 -36 -306 - 1077 MOTA C C 909 PHE 123 3.489 29.511 45.581 1.000 13.48 ANISOU 909 PHE 123 2004 1472 1645 157 1 8 236 ATOM 910 0 PHE 123 4.424 28.768 45.242 1.000 13.07 ANISOU 910 0 PHE 123 1591 1498 1876 42 - 78 - 172 ATOM 911 N ASP 124 3.294 30.684 44.948 1.000 13.83 ANISOU 911 N ASP 124 1490 1575 2189 51 207 2 8 8 MOTA CA ASP 912 124 4.207 31.036 43.861 1.000 13.75 ANISOU 912 CA ASP 124 1505 1330 2389 458 398 344 ATOM 913 СВ ASP 124 3.708 32.352 43.242 1.000 18.95 ASP ANISOU 913 СВ 124 2650 1970 2580 656 -63 926 ATOM 914 CG ASP 124 4.470 32.708 41.989 1.000 27.54 ANISOU 914 CG ASP 124 5327 2099 3036 -123 939 880 915 OD1 ASP 124 4.541 31.904 41.023 1.000 37.04 ANISOU 915 OD1 ASP 124 6362 3225 4485 108 2616 - 331

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ANISOU ATOM	U U U U J J J J J J J J J J J J J J J J	OCCOONNAA BBGGDDEEZZHH122 OCCOONNCCONNCCONNNN AABBGGDDEEEBBGGD	AGLN AGLN AGLN AGLN AGLN AGLN AGLN AGLN	122 122 122 122 122 122 122 122 122 122	7.214 7.214 7.396 7.396 7.396 7.3999 7.232 7.395 7.232 7.395 7.232 7.395 7.232 7.395 7	33.364 33.509 31.1721 31.30.64 11.30.63 11.21 11.30.63 11.27.18 11.2	4151 28 229.69 44 44 45 45 45 48 4 4 4 6 4 4 4 6 4 4 4 6 4 4 4 6 6 4 4 6 6 9 8 8 9 8 4 7 . 3 5 4 8 4 7 . 3 5 4 8 4 7 . 3 5 4 8 4 7 . 3 5 4 8 4 7 . 3 5 4 8 4 7 . 3 5 4 8 8 9 5 5 2 8 4 2 9 . 3 5 1 3 6 0 8 3 4 7 . 4 9 9 8 2 8 4 2 3 1 3 6 0 8 1 8 2 4 9 1 5 3 1 3 6 0 8 3 1 8 2 4 9 1 5 3 1 3 6 0 8 3 1 8 2 4 9 1 5 3 1 5 3 7 5 1 5 3 1 5	-1539 234 8 5 1 1.000 14.49 327 485 4 8 2 1.000 14.52 289 497 3 0 7 1.000 14.03 353 398 4 1 4 1.000 16.40 194 178 2 2 6 1.000 14.69 232 -25 15 3 1.000 14.10 7 -205 -201 1.000 18.13 787 -81 4 6 1.000 2 7.51 883 -36 -2 2 5 1.000 29.33 -667 237 -187 1.000 32.99 -678 -1642 1 5 6 1.000 27.38 -276 -580 -2 4 6 1.000 38.55 449 -2476 -669 1.000 3 8.55 449 -2476 -669 1.000 3 0.26 -369 -835 3 6 3 1.000 12.36 248 -63 -2 6 4 1.000 13.39 219 -355 -3 77 0.500 16.24 188 202 -1 9 2 0.500 18.83 68 233 -2 1 0 0.500 23.94 -604 -757 3 3 0.500 35.94 -578 -1567 -478 0.500 24.63 -881 -2407 4 6 2 0.500 13.36 602 -114 -255 0.500 18.28 -68 -176 -105
ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU	933 9334 934 935 935 936 937 937	CG CD CD OE1 NE2 NE2 CB	AGLN AGLN AGLN AGLN AGLN AGLN AGLN AGLN	126 126 126 126 126 126 126 126 126	2422 6.149 2761 7.077 3578 7.181 6788 7.774 4491 6.525 1695	1391 27.758 2021 27.146 2745 27.683 3731 26.055 1118 27.417 1137	2357 49.284 2371 50.298 2774 51.419 3136 50.008 3751 48.018 2245	188 202 - 192 0.500 18.83 68 233 - 210 0.500 23.94 -604 -757 3 3 0.500 35.94 -578 -1567 - 478 0.500 24.63 -881 -2407 462 0.500 13.36 602 -114 - 255
	939 939 940 941 942 943 944 944 945 945	CD CD OE1 NE2 C C O O N N C O O N C O O O O O O O O O	BGLN BGLN BGLN BGLN BGLN GLN GLN GLN TYR TYR TYR	126 126 126 126 126 126 126 127 127 127	2537 5.442 2227 5.605 3289 4 231		2153 50.319 2198 51.242 2828 50.003 4413 45.861 1979 45.748 1827 44.868 1735 43.585 1550	

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ATOM 947 CG TYR 127 5.791 25.069 41.496 1.000 11.49 ANISOU 948 CD1 TYR 127 1278 1428 1650 -4 -4 10 ATOM 948 CD1 TYR 127 6.550 24.928 41.270 1.000 11.28 ANISOU 949 CD1 TYR 127 6.406 24.153 40.115 1.000 11.28 ANISOU 950 CD2 TYR 127 1640 1167 2027 -51 -53 2 1 ANISOU 950 CD2 TYR 127 1677 1677 ATOM 951 CE2 TYR 127 4.871 25.655 39.47 204 -219 -10 0 ANISOU 951 CE2 TYR 127 4.771 25.655 39.357 1.000 11.47 ANISOU 951 CE2 TYR 127 4.771 25.655 39.357 1.000 11.57 ATOM 952 CZ TYR 127 1539 1118 1665 140 -68 -73 ANISOU 952 CZ TYR 127 1202 1226 1760 91.48 -125 ANISOU 952 CZ TYR 127 1202 1226 1760 91.48 -125 ANISOU 952 CZ TYR 127 1292 1226 1760 91.48 -125 ANISOU 953 OH TYR 127 1547 1138 1712 94.177 -3 ANISOU 955 OTYR 127 1296 989 1830 230 -43 3.78 ANISOU 955 O TYR 127 1292 12326 1003 164 -237 - 42 ANISOU 955 O TYR 127 1292 1232 1603 164 -237 - 42 ANISOU 956 N THR 128 1554 976 1642 212 -9 557 ANISOU 957 CA ANISOU 958 CB THR 128 1686 1125 1673 -47 -169 3 8 6 ANISOU 959 OGI THR 128 1873 1074 1864 -52 -233 5 2 1 ANISOU 950 OGI THR 128 1873 1074 1864 -52 -233 5 2 1 ANISOU 950 OGI THR 128 1873 1074 1864 -52 -233 5 2 1 ANISOU 950 OGI THR 128 1873 1074 1864 -52 -233 5 2 1 ANISOU 950 OGI THR 128 1873 1074 1864 -52 -233 5 2 1 ANISOU 950 OGI THR 128 1873 1074 1864 -52 -233 5 2 1 ANISOU 960 CG2 THR 128 10.878 31.500 41.893 1.000 10.26 6 ANISOU 961 C THR 128 1995 28.458 42.258 1.000 12.16 6 ANISOU 965 N ALA 129 1163 1001 17.63 70 -118 147 ANISOU 960 CG2 THR 128 1995 28.458 42.258 1.000 12.16 6 ANISOU 965 CB ALA 129 1273 28.868 45.037 1.000 10.59 9 ANISOU 960 CG ALA 129 1273 28.868 45.037 1.000 10.59 9 ANISOU 960 CG ALA 129 1273 28.868 45.037 1.000 10.99 3 ANISOU 960 CB ALA 129 1283 1995 28.468 42.258 1.000 12.16 6 ANISOU 960 CB ALA 129 1273 28.888 24.4504 1.000 10.99 3 ANISOU 960 CB ALA 129 1273 28.888 24.504 1.000 10.99 3 ANISOU 960 CB ALA 129 1273 28.888 24.504 1.000 10.99 3 ANISOU 960 CB ALA 129 1273 28.888 270 1.000 10.99 3 ANISOU 960 CB ALA 129 1273 28.888 28.2964 1.000 10.99 9 ANISOU 960 CB ALA 129 1273 28.888 28.2964 1.000 10.99 9 ANI	ANISOU	946	CB	TYR	127	1346	1655 1491 -13 82 4 7
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ATOM 970 CB ASER 130 10.342 23.940 44.716 0.500 10.08 ANISOU 970 CB ASER 130 1432 603 1793 213 247 413 ATOM 971 OG ASER 130 9.771 24.063 46.006 0.500 9.12 ANISOU 971 OG ASER 130 10.364 23.919 44.765 0.500 10.60 ANISOU 972 CB BSER 130 10.364 23.919 44.765 0.500 10.60 ANISOU 973 OG BSER 130 1687 822 1521 -45 318 158 ATOM 973 OG BSER 130 9.418 24.098 43.734 0.500 16.22 ANISOU 973 OG BSER 130 1717 1289 3156 137 -525 348 ANISOU 974 C SER 130 12.214 24.373 43.110 1.000 10.53 ANISOU 974 C SER 130 1586 733 1684 -166 210 484 ATOM 975 O SER 130 13.137 23.532 42.942 1.000 11.17 ANISOU 975 O SER 130 1385 1012 1849 -151 -95 140 ANISOU 976 N ARG 131 11.680 25.044 42.079 1.000 10.46						1623	876 1638 -85 44 3 7 0
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ATOM 972 CB BSER 130 10.21 651 1792 91 1 -143 ATOM 972 CB BSER 130 10.364 23.919 44.765 0.500 10.60 ANISOU 972 CB BSER 130 1687 822 1521 -45 318 1 5 8 ATOM 973 OG BSER 130 9.418 24.098 43.734 0.500 16.22 ANISOU 973 OG BSER 130 1717 1289 3156 137 -525 3 4 8 ATOM 974 C SER 130 12.214 24.373 43.110 1.000 10.53 ANISOU 974 C SER 130 1586 733 1684 -166 210 4 8 4 ATOM 975 O SER 130 13.137 23.532 42.942 1.000 11.17 ANISOU 975 O SER 130 1385 1012 1849 -151 -95 1 4 0 ATOM 976 N ARG 131 11.680 25.044 42.079 1.000 10.46							24.063 46.006 0.500 9.12
ANISOU 972 CB BSER 130 1687 822 1521 -45 318 158 ATOM 973 OG BSER 130 9.418 24.098 43.734 0.500 16.22 ANISOU 973 OG BSER 130 1717 1289 3156 137 -525 3 4 8 ATOM 974 C SER 130 12.214 24.373 43.110 1.000 10.53 ANISOU 974 C SER 130 1586 733 1684 -166 210 4 8 4 ATOM 975 O SER 130 13.137 23.532 42.942 1.000 11.17 ANISOU 975 O SER 130 1385 1012 1849 -151 -95 1 4 0 ATOM 976 N ARG 131 11.680 25.044 42.079 1.000 10.46				ASER	130		
ANISOU 972 CB BSER 130 1687 822 1521 -45 318 1 5 8 ATOM 973 OG BSER 130 9.418 24.098 43.734 0.500 16.22 ANISOU 973 OG BSER 130 1717 1289 3156 137 -525 3 4 8 ATOM 974 C SER 130 12.214 24.373 43.110 1.000 10.53 ANISOU 974 C SER 130 1586 733 1684 -166 210 4 8 4 ATOM 975 O SER 130 13.137 23.532 42.942 1.000 11.17 ANISOU 975 O SER 130 1385 1012 1849 -151 -95 1 4 0 ATOM 976 N ARG 131 11.680 25.044 42.079 1.000 10.46						10.364	23.919 44.765 0.500 10.60
ATOM 973 OG BSER 130 9.418 24.098 43.734 0.500 16.22 ANISOU 973 OG BSER 130 1717 1289 3156 137 -525 3 4 8 ATOM 974 C SER 130 12.214 24.373 43.110 1.000 10.53 ANISOU 974 C SER 130 1586 733 1684 -166 210 4 8 4 ATOM 975 O SER 130 13.137 23.532 42.942 1.000 11.17 ANISOU 975 O SER 130 1385 1012 1849 -151 -95 1 4 0 ATOM 976 N ARG 131 11.680 25.044 42.079 1.000 10.46				BSER	130	1687	
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ATOM 975 O SER 130 1586 733 1684 -166 210 484 ATOM 975 O SER 130 13.137 23.532 42.942 1.000 11.17 ANISOU 976 O SER 130 1385 1012 1849 -151 -95 140 ATOM 976 N ARG 131 11.680 25.044 42.079 1.000 10.46							24.373 43.110 1.000 10.53
ATOM 975 O SER 130 13.137 23.532 42.942 1.000 11.17 ANISOU 975 O SER 130 1385 1012 1849 -151 -95 140 ATOM 976 N ARG 131 11.680 25.044 42.079 1.000 10.46					130	1586	733 1684 -166 210 484
ANISOU 975 O SER 130 1385 1012 1849 -151 -95 140 ATOM 976 N ARG 131 11.680 25.044 42.079 1.000 10.46							23.532 42.942 1.000 11.17
ATOM 976 N ARG 131 11.680 25.044 42.079 1.000 10.46							1012 1849 -151 -95 140
							25.044 42.079 1.000 10.46
	MILZOU	7/0	N	ARG	131	1578	

- 122 -MOTA 977 CAARG 131 12.260 24.839 40.742 1.000 10.60 ANISOU 977 CA131 1480 ARG 1110 1438 61 - 288 8 2 MOTA 978 CВ ARG 131 11.426 25.553 39.679 1.000 12.99 ANISOU 978 CB 131 1893 ARG 1369 1673 63 - 525 276 979 ATOM CG ARG 131 10.003 25.065 39.431 1.000 13.64 ANISOU 979 CG ARG 131 1707 1735 1742 -559 - 86 335 MOTA 980 CD ARG 131 9.349 25.669 38.206 1.000 17.71 ANISOU 980 CD ARG 131 2078 1973 2677 81 - 983 701 MOTA 981 ARG ΝE 131 9.453 27.113 38.015 1.000 19.76 ANISOU 981 ΝĒ ARG 131 2716 2034 2757 -25 -525 7 1 3 ARG 131 8.629 MOTA 982 CZ28.004 38.568 1.000 21.24 ANISOU 982 CZARG 131 3688 1878 -8 -128 647 2503 983 MOTA NH1 ARG 131 7.631 27.634 39.366 1.000 21.32 ANISOU 983 NH1 AEG 131 2792 3142 2166 -486 -667 5 7 984 NH2 ARG ATOM 131 8.771 29.310 38.361 1.000 27.83 ANISOU 984 NH2 ARG 131 4649 1822 4103 -90 -422 5 6 1 985 ATOM ARG 131 13.714 C 25.323 40.688 1.000 10.42 ANISOU 985 С ARG 131 1542 1078 1339 50 -103 ATOM 986 0 ARG 131 14.568 24.683 40.080 1.000 10.94 ANISOU 986 0 ARG 131 1544 1105 177 -134 4 2 1506 ATOM 987 ALA 132 14.028 N 26.438 41.343 1.000 10.97 ANISOU 987 ALA 132 1477 Ν 1129 1563 74 - 364 - 45 ALA 132 15.379 ATOM 988 CA 26.983 41.343 1.000 11.10 ANISOU 988 CA ALA 132 1539 944 1735 9 -102 9 7 ATOM 989 CB ALA 132 15.429 28.344 42.048 1.000 12.82 ANISOU 989 ALA 132 1711 CB 1171 1987 -48 -248 - 198MOTA 990 С ALA 132 16.393 26.045 41.995 1.000 11.55 ANISOU 990 С 132 1085 1107 2197 -197 305 7 132 17.481 25.832 41.432 1.000 11.81 ALA-197 305 745 MOTA 991 0 ALA 132 1081 1809 1599 -204 17 - 9 133 16.061 25.490 43.175 1.000 11.16 ANISOU 991 0 ALA 992 N ATOM VAL ANISOU 992 VAL 133 1260 N 1356 1623 -148 51 3 5 0 VAL 133 17.011 24.587 43.840 1.000 11.62 ATOM 993 CAANISOU 993 CAVAL 133 1505 1529 1380 -69 -297 8 9 VAL 133 16.738 24.418 45.344 1.000 12.14 MOTA 994 CB ANISOU 994 CB VAL 133 1376 1674. 1564 -74 -25 364 995 CG1 VAL 133 15.550 23.501 45.608 1.000 14.96 ATOM ANISOU 995 CG1 VAL 133 1705 133 1705 2316 1662 -706 8 -357 133 17.981 23.864 46.033 1.000 15.63 2316 MOTA 996 CG2 VAL ANISOU 996 CG2 VAL 133 1755 2340 1845 -341 -677 5 5 1 997 ATOM VAL 133 17.079 23.268 43.065 1.000 11.71 С ANISOU 997 С VAL 133 1376 1363 1711 -24 -425 1 6 9 998 O ATOM VAL 133 18.198 22.733 42.925 1.000 11.55 ANISOU 998 0 VAL 133 1391 1453 1545 -4 -116 398 ATOM 999 N ALA 134 15.982 22.758 42.480 1.000 12.87 ANISOU 999 N ALA 134 1399 1517 1973 28 - 334 - 228 MOTA 1000 CA ALA 134 16.084 21.557 41.621 1.000 10.57 ANISOU 1000 CA ALA 134 1106 1220 1691 153 -298 9 6 MOTA 1001 CB ALA 134 14.699 21.096 41.186 1.000 12.20 ANISOU 1001 CB ALA 134 1254 1589 1794 35 - 303 - 127 ATOM 1002 C ALA 134 16.968 21.797 40.399 1.000 12.58 ANISOU 1002 C ALA 134 1393 1399 1987 272 -4 2 7 7 MOTA 1003 0 ALA 134 17.712 20.924 39.970 1.000 11.01 ANISOU 1003 O ALA 134 1254 1358 1574 83 - 268 2 6 MOTA 1004 N ARG 135 16.908 22.995 39.809 1.000 12.03 ANISOU 1004 N 135 1517 ARG 1230 1824 -62 -327 8 7 MOTA 1005 CA ARG 135 17.773 23.353 38.676 1.000 13.23 ANISOU 1005 CA 135 1854 ARG 1158 2015 -270 -209 1 6 1 ATOM 1006 CB ARG 135 17.393 24.734 38.170 1.000 14.57 ANISOU 1006 CB ARG 135 2203 1339 1994 -45 -541 2 2 2 1007 CG MOTA ARG 135 17.753 25.160 36.797 1.000 19.22

ANISOU 1007 CG ARG 135 4204 1120 1980 -490 -433 150 ATOM 1008 CD ARG 135 17.237 26.563 36.471 1.000 22.14 ANISOU 1008 CD ARG 135 4046 1500 2868 -159 315 822 ATOM 1009 NE ARG 135 15.831 26.607 36.077 1.000 22.66 ANISOU 1009 NE ARG 135 4239 1404 2965 -94 47 257 ATOM 1010 CZ ARG 135 14.802 27.184 36.684 1.000 21.69 ANISOU 1010 CZ ARG 135 4004 1906 2333 92 -506 6 4 ATOM 1011 NH1 ARG 135 14.917 27.843 37.833 1.000 22.26 ANISOU 1011 NH1 ARG 135 4114 2532 1812 460 -833 34 1 ATOM 1012 NH2 ARG 135 13.582 27.113 36.149 1.000 22.31 ANISOU 1012 NH2 ARG 135 4000 2243 2234 -544 -419 8 - 123 -ANISOU 1012 NH2 ARG 135 4000 2243 2234 -544 -419 8
ATOM 1013 C ARG 135 19.251 23.275 39.057 1.000 12.70
ANISOU 1013 C ARG 135 1742 1264 1821 -119 -16 4
ATOM 1014 O ARG 135 20.069 22.818 38.238 1.000 14.67
ANISOU 1014 O ARG 135 2133 1529 1910 19 169 3 9 1
ATOM 1015 N GLU 136 19.572 23.712 40.266 1.000 12.15
ANISOU 1015 N GLU 136 1423 1372 1820 -36 70 4 3 0
ATOM 1016 CA GLU 136 20.960 23.630 40.763 1.000 14.52
ANISOU 1016 CA GLU 136 1622 1701 2194 -90 -197 3
ATOM 1017 CB GLU 136 21.212 24.513 41.981 1.000 15.59
ANISOU 1017 CB GLU 136 1502 1781 2642 14 -231 1 1 -544 -419 8 -119 -16 430 -36 70 4 3 0 -90 -197 3 7 1 1017 CB GLU 136 1502 1781 2642 14 -231 1 1 1018 CG GLU 136 21.064 26.020 41.783 1.000 18.01 ANISOU 1017 CB GLU 136 1502 ATOM ANISOU 1018 CG GLU 136 2010 1018 CG GLU 136 2010 1/62 30/1 -232 -133 1 1019 CD GLU 136 21.798 26.484 40.537 1.000 20.18 1762 -232 -153 1 2 6 ATOM ANISOU 1019 CD GLU 136 2071 2079 3519 -308 89 3 6 9 1020 OE1 GLU 136 22.987 26.148 40.394 1.000 24.64 ATOM ANISOU 1020 OE1 GLU 136 2060 2937 4364 -262 338 615 1021 OE2 GLU 136 21.195 27.150 39.670 1.000 24.19 ANISOU 1021 OE2 GLU 136 2479 2327 4385 -381 317 1426 ATOM 1022 C GLU 136 21.364 22.186 41.076 1.000 14.00 14.00 ANISOU 1022 C GLU 136 1338 1619 2361 -112 -442 2 2 3 ATOM 1023 O GLU 136 1366 1890 2009 -100 -287 3 2 9 ATOM 1024 N VAL 137 20.472 21.338 41.580 1.000 11.78 ANISOU 1024 N VAL 137 1309 1451 1715 148 -223 8 5 ATOM 1025 CA VAL 137 20.472 ANISOU 1025 CA VAL 137 1369 1522 1853 240 -69 2 8 9 ATOM 1026 CB VAL 137 1369 1522 1853 240 -69 2 8 9 ATOM 1026 CB VAL 137 1422 1424 1869 -67 -85 -204 ANISOU 1027 CG1 VAL 137 19.560 19.165 42.429 1.000 12.41 ANISOU 1027 CG1 VAL 137 19.728 17.634 42.401 1.000 12.55 ANISOU 1027 CG1 VAL 137 19.355 ANISOU 1028 CG2 VAL 137 1461 1281 1572 182 -254 2 8 8 ATOM 1029 C VAL 137 1202 1428 2113 150 -16 8 5 ATOM 1030 O VAL 137 1202 1428 2113 150 -16 8 5 ATOM 1030 O VAL 137 1202 1428 2113 150 -16 8 5 ATOM 1031 N LEU 138 1198 ANISOU 1031 N LEU 138 ANISOU 1021 OE2 GLU 136-2479 2327 4385 1031 N LEU 138 1198 881 1829 -15 158 2 2 6 1032 CA LEU 138 20.571 19.029 38.066 1.000 12.48 ATOM ANISOU 1032 CA LEU 138 1312 1032 CA LEU 138 1312 1408 2024 110 273 - 5 2 1033 CB LEU 138 19.398 19.358 37.130 1.000 11.81 MOTA ANISOU 1033 CB LEU 138 1260 1586 1642 -20 383 4 3 LEU 138 18.036 18.726 37.457 1.000 10.77 ATOM 1034 CG ANISOU 1034 CG LEU 138 1391 1034 CG LEU 138 1391 1397 1304 -83 219 2 1 3 1035 CD1 LEU 138 16.916 19.324 36.596 1.000 12.72 ANISOU 1035 CD1 LEU 138 1416 1035 CD1 LEU 138 1416 1587 1829 -59 -25 173 1036 CD2 LEU 138 18.052 17.207 37.320 1.000 14.32 ANISOU 1036 CD2 LEU 138 1986 1390 2065 - 79 296 370 1037 C LEU 138 21.903 19.525 37.505 1.000 13.61 ANISOU 1037 C LEU 138 1305 2026 1840 -65 174 5

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1038 0
                     LEU 138 22.695
                                            18.760 36.920 1.000 14.97
ANISOU 1038 O
                     LEU
                            138 1125
                                                                         234 178
                                            2247
                                                       2313
                                                                 105
         1039 N
                                            20.816 37.614 1.000 13.26
ATOM
                     ARG
                           139 22.184
ANISOU 1039 N
                           139 1432
                     ARG
                                                                        219 317
                                            2046
                                                       1561
                                                                 -155
         1040 CA ARG 139 23.397
                                            21.372 37.085 1.000 14.71
ATOM
ANISOU 1040 CA ARG
                           139 1648
                                            1941
                                                       2000
                                                                 -27
                                                                         502 447
         1041 C
                     ARG
                           139 24.636
                                            20.815 37.775 1.000 15.16
ATOM
ANISOU 1041 C
                     ARG 139 1425
                                            2101
                                                      2235
                                                                 -158 324 116
         1042 0
ATOM
                     ARG 139 25.650
                                            20.495 37.166 1.000 18.15
ANISOU 1042 O
                                                                 18 612 3 3 9
                     ARG 139 1628
                                            2581
                                                      2688
         1043 CB ARG 139 23.394
                                            22.926 37.206 1.000 19.67
ATOM
ANISOU 1043 CB ARG 139 1749
                                            1923
                                                      3803
                                                                 -196 186 252
         1044 CG
                    ARG 139 24.418
                                            23.487 36.237 1.000 28.66
ATOM
ANISOU 1044 CG
                    ARG 139 3924
                                            2584 4383
                                                                -2305 882 - 563
         1045 CD ARG 139 24.245
                                            24.997 36.111 1.000 39.58
ANISOU 1045 CD ARG 139 6801
                                            2389
                                                     5849
                                                                -3273 119 - 306
         1046 NE
                    ARG 139 24.910 25.660 37.210 1.000 47.91
ATOM
                    ARG 139 9548 2435 6222 -2157 -1331
ARG 139 24.493 26.682 37.928 1.000 45.42
ANISOU 1046 NE
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ATOM
         1047 CZ
ATOM 1047 CZ ARG 139 24.493 26.682 37.928 1.000 45.42

ANISOU 1047 CZ ARG 139 6941 4516 5802 -882 -2118 -

ATOM 1048 NH1 ARG 139 23.316 27.273 37.722 1.000 64.33

ANISOU 1048 NH1 ARG 139 7248 8153 9039 93 -2965 -98

ATOM 1049 NH2 ARG 139 25.309 27.109 38.888 1.000 32.62

ANISOU 1049 NH2 ARG 139 5020 4758 2616 -2746 590 1 ATOM 1050 N ALA 140 24.562 20.684 39.096 1.000 14.85

ANISOU 1050 N ALA 140 1287 2204 2151 -517 -26 -

ATOM 1051 CA ALA 140 25.730 20.257 39.856 1.000 15.80

ANISOU 1051 CA ALA 140 989 2649 2366 -309 -9 -401

ATOM 1052 CB ALA 140 2685 2447 2222 243 -435 -4

ATOM 1053 C ALA 140 2685 2447 2222 243 -435 -4

ATOM 1053 C ALA 140 2685 2447 2222 243 -435 -4
                                                                 -882 -2118 -1238
                                                                 93 -2965 - 980
                                                                 -2746 590 1 6 7
                                                                 -517 -26 - 46
                                                                 243 -435 - 480
         1053 C
                     ALA 140 26.111 18.806 39.584 1.000 16.86
                     ALA 140 1555 2795
ANISOU 1053 C
                                                      2054
                                                                 12 - 186 - 458
MOTA
         1054 O
                     ALA 140 27.258 18.403 39.796 1.000 18.90
ANISOU 1054 O
                      ALA 140 1538 2686
                                                      2958
                                                                 -21
                                                                       60 1 4 5
                     THR 141 25.147 18.025 39.098 1.000 17.53
MOTA
         1055 N
ANISOU 1055 N
                     THR 141 1779 2532
                                                       2350
                                                                 -528 218 -108
MOTA
         1056 CA THR 141 25.340 16.625 38.765 1.000 15.59
ANISOU 1056 CA
                     THR 141 1256 2401
                                                       2268
                                                                 -192 -95 291
ATOM
         1057 CB
                     THR 141 24.207 15.735 39.343 1.000 14.77
ANISOU 1057 CB
                     THR 141 1238 2200
                                                       2172
                                                                 155
                                                                         282 3 0 1
          1058 OG1 THR 141 22.946 16.168 38.849 1.000 12.47
MOTA
ANISOU 1058 OG1 THR 141 1249 1565 1926 -31 295 4
ATOM 1059 CG2 THR 141 24.167 15.818 40.859 1.000 14.82
                                                                 -31 295 476

    141 1394
    2077
    2160
    135
    -47
    1

    141 25.423
    16.374
    37.257
    1.000
    16.11

ANISOU 1059 CG2 THR
                                                                        -47 177
MOTA
          1060 C
                      THR
ANISOU 1060 C

    141
    1732
    2046
    2343
    303
    583
    3

    141
    25.432
    15.235
    36.778
    1.000
    17.55

                      THR
                                                                         583 325
          1061 0
ATOM
                      THR

    141
    1991
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    555
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    36.446
    1.000
    17.74

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    2197
    2416
    303
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    142
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    17.263
    34.987
    1.000
    17.32

ANISOU 1061 O
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          1062 N
 ATOM
                      GLY
ANISOU 1062 N
                                                                               501
                      GLY
 MOTA
          1063 CA
                      GLY
                            142 1642
 ANISOU 1063 CA
                      GLY
                                                                  -160 453 517
                                             2494
                                                       2447
                            142 24.426 16.556 34.358 1.000 16.37
          1064 C
                      GLY
 ANISOU 1064 C
                      GLY
                            142 1619
                                             1893
                                                                        472 4 2
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          1065 O
                      GLY
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 ANISOU 1065 O
                      GLY
                            142 2243
                                             2558
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                                                       2201
          1066 N
                      THR
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 ANISOU 1066 N
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                                                                  83 430 3 5 0
                      THR
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          1067 CA
                      THR
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 ANISOU 1067 CA
                      THR 143 1768
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 ATOM
          1068 CB
                      THR
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- 125 -

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ATOM 1069 OG1 THR 143 1457 1653 2785 55 419 5 2 9
ANISOU 1069 OG1 THR 143 22.037 14.784 36.573 1.000 14.63
ATOM 1070 CG2 THR 143 1296 1792 2471 52 424 2 CG
         ANISOU 1068 CB THR 143 1457
                                      THR 143 1761 1981 1669 3 379 192
THR 143 21.135 16.785 33.532 1.000 13.96
THR 143 1553 1708 2044 122
        ANISOU 1070 CG2 THR 143 1761
        ATOM
                                     1071 C
      ANISOU 1071 C THR 143 21.135 16.785 33.532 1.000 13.96
ANISOU 1072 O THR 143 20.642 17.828 33.923 1.000 15.65
ANISOU 1072 O THR 143 2374 1580 1995 315 486 5
ATOM 1073 N GLU 144 20.928 16.279 32.322 1.000 15.32
ANISOU 1073 N GLU 144 1734 1904 2184 -156 260 -2
ANISOU 1074 CA GLU 144 19.917 16.693 31.362 1.000 17.30
ANISOU 1074 CA GLU 144 1686 2470 2417 -377 152 16
                                                                                                                                                                                                                                                                                                     479 - 131
                                                                                                                                                                                                                                                                            315 486 5 5
ATOM 1074 CA GLU 144 1734 1904 1816 1000 17.30 ANISOU 1074 CA GLU 144 1686 2470 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.30 17.3
                                                                                                                                                                                                                                                                            -156 260 -271
                                                                                                                                                                                                                                                                            -2037 -2082 1767
                                                                                                                                                                                                                                                                          -2497 -2259 2129
                                                                                                                                                                                                                                                                          -595 -1282 - 323

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    3484
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    419
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    147
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    27.155
    1.000
    18.06

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    2451
    1638
    -382
    98
    9

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                                           1098 CA GLY
      ANISOU 1098 CA
                                                                                           GLY
                                                                                                                                                                                    2451
                                                                                                                                                                                                                             1638
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- 126 -GLY 147 13.361 17.574 27.609 1.000 18.73 ATOM 1099 C ANISOU 1099 C GLY 147 2836 147 12.676 18.570 27.282 1.000 18.34 147 2865 2416 1687 -524 143 527 1100 O GLYANISOU 1100 O GLY 2416 1687 -413 -72 389 1101 N GLY148 14.498 17.634 28.316 1.000 16.35 ANISOU 1101 N GLY 148 2936 1506 1772 -157 142 8 8 1102 CA 148 15.116 18.889 28.747 1.000 15.34 GLY148 2723 1279 1829 55 450 - 26 148 14.768 19.339 30.144 1.000 12.97 ANISOU 1102 CA GLY ATOM 1103 C GLY ANISOU 1103 C
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 1416
 1280
 -93
 -62
 4

 148 13.769
 18.930
 30.771
 1.000
 13.79
 GLY -93 -62 4 0 7 1104 0 ATOM GLY ANISOU 1104 O GLY 148 2301 1376 1561 149 15.604 20.224 30.718 1.000 12.81 -164 88 3 2 3 1105 N ATOM VAL ANISOU 1105 N VAL 149 1815 1366 1686 155 -31 238 1106 CA 149 15.388 20.724 32.079 1.000 11.81 MOTA VAL ANISOU 1106 CA VAL 149 1333 1390 1765 54 -92 1 2 9 21.636 32.480 1.000 11.97 MOTA 1107 CB VAL 149 16.594 ANISOU 1107 CB 1107 CB VAL 149 1136 1696 1717 -100 246 1 1108 CG1 VAL 149 16.358 22.336 33.802 1.000 15.26 -100 246 124 ATOM ANISOU 1108 CG1 VAL 149 1941 1922 1936 -195 55 - 223 1109 CG2 VAL 149 17.868 20.794 32.538 1.000 17.21 MOTA ANISOU 1109 CG2 VAL 149 1231 2045 3265 45 102 -103 ATOM 1110 C 149 14.101 21.482 32.280 1.000 11.32 VAL VAL 149 1186 1303 1813 -78 131 4
VAL 149 13.378 21.218 33.253 1.000 12.35
VAL 149 1664 1423 1608 -71 229 1
GLU 150 13.752 22.463 31.460 1.000 11.96 ANISOU 1110 C 131 479 ATOM 1111 0 ANISOU 1111 O -71 229 167 ATOM 1112 N GLU 150 1347 1453 1746 29 -36 420 GLU 150 12.592 23.286 31.815 1.000 10.90 ANISOU 1112 N MOTA 1113 CA ANISOU 1113 CA GLU 150 1623 1359 1159 118 0 405 GLU 150 12.608 24.601 30.999 1.000 17.60 ATOM 1114 CB ANISOU 1114 CB GLU 150 2530 1470 2687 181 -161 9 0 7 25.488 31.314 1.000 17.86 ATOM 1115 CG GLU 150 13.811 ANISOU 1115 CG GLU 150 2744 797 3246 246 434 202 GLU 150 13.956 25.929 32.738 1.000 19.47 ATOM 1116 CD ANISOU 1116 CD GLU 150 3018 1353. -97 -84 662 3027 ATOM 1117 OE1 GLU 150 12.951 26.005 33.475 1.000 18.21 ANISOU 1117 OE1 GLU 150 3035 1512 2373 -178 -321 5 -178 -321 5 3 6 ATOM 1118 OE2 GLU 150 15.109 26.237 33.122 1.000 22.59 ANISOU 1118 OE2 GLU 150 2993 1664 3927 -38 -150 2 8 4 ATOM 1119 C 150 11.277 22.533 31.705 1.000 12.22 GLU ANISOU 1119 C GLU 150 1429 1540 1676 235 147 - 5 1120 O GLU 150 10.341 22.757 32.530 1.000 13.44 GLU ANISOU 1120 O 150 1739 1474 1894 315 470 288 ATOM 1121 N ALA 151 11.118 21.625 30.742 1.000 11.88 ANISOU 1121 N ALA 151 1783 1255 1477 94 45 253 ATOM 1122 CA ALA 151 9.881 20.844 30.698 1.000 13.82 ANISOU 1122 CA ALA 151 1744 ATOM 1123 CB ALA 151 9.739 2054 1454 -100 -413 3 9 6 20.094 29.390 1.000 14.89 ANISOU 1123 CB ALA 151 1489 2318 1851 22 - 269 - 35 ATOM 1124 C ALA 151 9.792 19.864 31.867 1.000 12.71 ANISOU 1124 C ALA 151 1448 1463 1920 93 41 4 2 4 1125 0 MOTA ALA 151 8.655 19.580 32.280 1.000 14.69 ANISOU 1125 O 151 1535 ALA2114 1932 -242 204 - 108ATOM 1126 N PHE 152 10.925 19.401 32.410 1.000 11.73 ANISOU 1126 N PHE 152 1598 1259 1598 120 ATOM 1127 CA PHE 152 10.890 18.554 33.602 1.000 10.61 ANISOU 1127 CA PHE 152 1444 1061 1526 -33 34 1 6 0 ATOM 1128 CB PHE 152 12.293 17.981 33.820 1.000 10.23 ANISOU 1128 CB PHE 152 1317 1132 1437 -144 207 410 1129 CG PHE 152 12.517 17.187 35.095 1.000 10.36 ATOM

						- 127 -		
ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU ANI	1131 1132 1133 1133 1133 1133 1133 1133	CCCCCCCCCOONN CCCBGGDDD22 CCCCCCCCCOONN CCCBGGDDD22 CCCCCCCCCCCOONN CCCBGGDDD22	PPPPPPPPPPPPPPPPPPPPPPPPPPPPPPPPPPPPPP	1522222222222333333333333333344444444444	13.29 1489 12.252 13.431 1709 165.130 17548 165.280 17548 165.809 10	1149 15.896 1047.701 145.14.16.123.49 16.2271.60.22 15.04.99.16.87.22 116.8.72.71 19.68.72.72 110.68.72.73 121.22.42.13 121.23.8.19.10 121.23.8.91.0 121.23.8.91.0 121.23.8.91.0 121.23.8.91.0 121.23.8.91.0 121.23.8.91.0 121.23.8.91.0 121.23.91.0 1	3110 34.985 1265	-34 147 276 1.000 11.24 114 -103 566 1.000 11.21 85 174 151 1.000 10.80 249 -111 373 1.000 11.82 -276 414 250 1.000 12.24 -10 339 8 4 1.000 12.24 -10 339 8 4 1.000 11.49 200 109 277 1.000 11.86 -673 156 1.000 11.99 -165 307 85 1.000 12.81 -72 97 - 40 1.000 12.87 146 269 6 4 1.000 15.99 -49 450 - 431 1.000 15.99 -49 450 - 431 1.000 19.37 809 275 540 1.000 12.96 -336 360 - 43 1.000 13.24 -443 481 - 182 1.000 13.29 60 517 280 1.000 13.29 60 517 280 1.000 13.29 60 517 280 1.000 13.29 60 517 280 1.000 13.29 60 517 280 1.000 13.29 60 517 280 1.000 13.29 60 517 280 1.000 13.29 60 517 280 1.000 13.29 60 517 280 1.000 13.29 60 517 280 1.000 13.29 60 517 280 1.000 13.29 60 517 280 1.000 13.29 60 517 280 1.000 13.29 60 517 280 1.000 13.29 60 517 280 1.000 22.95 676 430 1501 1.000 24.33 228 48 1128 1.000 24.33 228 48 1128 1.000 11.22 123 147 4 1 0
ANISOU ATOM ANISOU ATOM	1145 1146 1146 1147	N CA CA CB	ASP ASP ASP ASP	154 154 154 154 154	8.568 1643 7.195 1862 6.995	22.203 1457 22.671 1255 23.269	34.955 1951 34.764 2280 33.373	1.000 13.29 60 517 2 8 0 1.000 14.21 313 631 6 8 3
ATOM ANISOU ATOM ANISOU ATOM	1148 1148 1149 1149 1150	CG CG OD1 OD1 OD2	ASP ASP ASP ASP	154 154 154 154	5.534 2323 4.685 2164	23.367 3543 23.607 2368	32.929 2855 33.820 3389	1.000 22.95 676 430 1501 1.000 20.85 895 478 1144
ATOM ANISOU ATOM ANISOU ATOM	1151 1151 1152 1152 1153	C C O O N	ASP ASP ASP ASP CYS	154 154 154 154 155	2989 6.294 1594 6.043 2143 5.891	3146 21.455	3110 34.985	228
ANISOU ATOM ANISOU ATOM ANISOU ATOM	1154 1154 1155 1155 1156	CA CA CB CB SG	CYS CYS CYS CYS CYS	155 155 155 155 155	1425 5.446 1294 6.635 1276 7.316	1098 19.881 1168 19.171 1015 19.819	1243	-76 186 2 7 1.000 9 . 4 1 -13 154 1 7 2 1.000 10 . 6 4 28 -51 - 1 2 2 1.000 12 . 0 1
ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU	1157 1157 1158 1158 1159	SCCOONN	CYS CYS CYS CYS GLU GLU	155 155 155 155 156	1376 4.138 1301 3.215 1349 4.021 1263	1554 19.885 1355 20.645 1386 19.033	1633 37.423 1013 37.064 1676 38.442	-195 -199 9 5 1.000 9.66 115 146 2 1 6 1.000 11.61 130 116 2 9 4 1.000 10.26
			220	1 J	1200	1495	1139	-29 168 299

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ATOM
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                 GLU
ANISOU 1161 CB
                 GLU
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MOTA
       1162 CG
                 GLU
ANISOU 1162 CG
                 GLU
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       1163 CD
                 GLU
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ANISOU 1163 CD
                GLU
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ANISOU 1164 OE1 GLU
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3269 2653 -243 -721 9
       1165 OE2 GLU
                      156 0.136
ANISOU 1165 OE2 GLU
                      156 2449
                                                     -243 -721 9 2 4
       1166 C
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1135 1197 -26 239 1
ATOM
                 GLU
                      156 2.961
ANISOU 1166 C
                 GLU
                      156 1166
                                                           239 183
       1167 O
ATOM
                 GLU
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ANISOU 1167 O
                 GLU
                      156 1631
                                   1199
                                            1434
                                                     103
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ATOM
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                PRO 157 1329 1201 1381 -109 21 1 2 3
PRO 157 3.527 21.407 40.359 1.000 10.17
PRO 157 1381 1093 1391 -40 -30 2
ANISOU 1168 N
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ATOM
ANISOU 1169 CD
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ATOM
ANISOU 1172 CG
ATOM 1173 C
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ANISOU 1173 C
                 PRO
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       1174 0
ATOM
                 PRO
ANISOU 1174 O
                 PRO
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ATOM
       1175 N
                 LEU
ANISOU 1175 N
                 LEU
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ATOM
                LEU
ANISOU 1176 CA
                LEU
       1177 CB
                 LEU
ANISOU 1177 CB
                 LEU
ATOM
       1178 CG
                 LEU
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2249 2685 -111 41 -23
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ANISOU 1179 CD1 LEU 158 1224
       11/9 CD1 LEU 158 1224 2249 2685 -111 41 -239 1180 CD2 LEU 158 -0.086 16.736 47.397 1.000 17.17
ATOM
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ANISOU 1181 C
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ANISOU 1182 O
                 LEU
ATOM
       1183 N
                 LEU
ANISOU 1183 N
                 LEU
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ATOM
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ANISOU 1184 CA
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                 LEU
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ANISOU 1186 CG LEU 159 1600
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ATOM
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        1190 O
                  LEU
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ATOM
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ANISOU 1194 CG
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                    ARG
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         1195 CD
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ATOM
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ANISOU 1200 C
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ANISOU 1201 O
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                         160 1291 3411 1791 -400 74 -81 161 -0.258 22.369 54.114 1.000 14.95
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ANISOU 1202 N PHE 161 1512
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ANISOU 1203 CA PHE 161 1600
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ATOM
ANISOU 1204 CB PHE 161 1594
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ANISOU 1205 CG PHE 161 2464 2424 3684 -39 790 -
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        1206 CD1 PHE 161 -1.175 25.010 57.849 1.000 26.03
ANISOU 1206 CD1 PHE 161 3353 2919
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ATOM 1207 CD2 PHE 161 0.822 25.901 56.885 1.000 25.34 ANISOU 1207 CD2 PHE 161 2353 3265 4011 -179 -161 -
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ATOM 1208 CE1 PHE 161 -0.943 25.660 59.051 1.000 30.50 ANISOU 1208 CE1 PHE 161 4784 3324 3481 -972 1456 -6 ATOM 1209 CE2 PHE 161 1.061 26.553 58.080 1.000 26.10
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ATOM
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ANISOU 1210 CZ
ATOM
        1211 C
ANISOU 1211 C
        1212 0
ANISOU 1212 O
ATOM
        1213 N
                         162 2063 2516 1610 -937 -523 7 7 162 -0.635 20.719 58.483 1.000 15.62
ANISOU 1213 N
                   ARG
ATOM
        1214 CA ARG
ANISOU 1214 CA ARG
                         162 1772
                         162 1772 2512 1650 -519 -266 7 6
162 -0.476 21.312 59.890 1.000 17.48
ATOM
        1215 C
                   ARG
ANISOU 1215 C
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162 0.609
                   ARG
                                        3131 1656 -603 -186 - 76
21.734 60.251 1.000 17.23
ATOM
        1216 0
                   ARG
ANISOU 1216 O
                                      3063 1557 -771 -42 -160
19.374 58.458 1.000 21.99
2318 2727
                   ARG 162 1928
ATOM
        1217 CB ARG 162 0.081
ANISOU 1217 CB ARG 162 3309
                                        2318
                                                  2727 -272 -737 - 22
MOTA
        1218 CG ARG 162 -0.573 18.322 59.348 1.000 26.07
ANISOU 1218 CG
                  ARG
                         162 3488
                         162 3488 2375 4041 489 655 280
162 -0.231 16.896 58.886 1.000 25.85
                                        2375
ATOM
        1219 CD
                   ARG
ANISOU 1219 CD
                   ARG
                         162 3106
                         162 3106 2221 4495 418 -2 2 3 9
162 -0.943 15.916 59.698 1.000 28.83
        1220 NE
ATOM
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ANISOU 1220 NE
                   ARG 162 4379
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ARG 162 -0.642 14.638 59.879 1.000 27.99
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 ANISOU 1221 CZ
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                                           3863
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 MOTA
        1222 NH1 ARG
                      162 0.429
                                   14.119 59.273 1.000 26.61
 ANISOU 1222 NH1 ARG
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                                           3742
                                   3167
                                                   -91
                                                        -126 - 268
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162 3807 3522 5663 -986 702 7
163 -1.570 21.296 60.622 1.000 16.77
 ATOM
        1223 NH2 ARG
 ANISOU 1223 NH2 ARG
                                                  -986 702 780
 ATOM
        1224 N
                 TYR
 ANISOU 1224 N
                 TYR
                      163 1803
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                                                  -484 -1948 4
        1225 CA
 MOTA
                 TYR
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 ANISOU 1226 CB
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 ANISOU 1227 CG
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 MOTA
 ANISOU 1228 CD1 TYR
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       1229 CE1 TYR
ANISOU 1229 CE1 TYR
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       1230 CD2 TYR
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ANISOU 1231 CE2 TYR
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                TYR
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ANISOU 1232 CZ
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ANISOU 1233 OH
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                                                  -269 1801 - 3052
                 TYR 163 -1.935 20.551 62.896 1.000 17.90
TYR 163 2872 2353 1575 -894 -465 -:
TYR 163 -2.933 19.858 62.653 1.000 18.12
ATOM
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ANISOU 1234 C
                                                  -894 -465 - 173
MOTA
       1235 O
ANISOU 1235 O
                 TYR
                     163 2694
                                  2130
                                          2060
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       1236 N
ATOM
                     164 -1.112 20.326 63.898 1.000 18.32
164 2516 2621 1826 -614 -402 -
                 PHE
ANISOU 1236 N
                 PHE
                                                  -614 - 402 - 90
       1237 CA
ATOM
                PHE
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ANISOU 1237 CA
                PHE
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                                          2038
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ANISOU 1238 CB
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ATOM
       1239 CG
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ANISOU 1239 CG
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                PHE
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ATOM
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ANISOU 1240 CD1 PHE
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MOTA
       1241 CD2 PHE
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ANISOU 1241 CD2 PHE
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ANISOU 1242 CE1 PHE
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ANISOU 1243 CE2 PHE
                     164 4719
                                  3694
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                                                  -293 657 -383
MOTA
       1244 CZ
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ANISOU 1244 CZ
                PHE
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                                  3808
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ATOM
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ANISOU 1245 C
                 PHE
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ATOM
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ANISOU 1246 O
                 PHE
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ATOM
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                 PRO
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                PRO
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ANISOU 1250 O
                 PRO
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MOTA
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                 PRO
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ANISOU 1251 CB PRO 165 3640
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  ATOM 1252 CG PRO 165 -5.417 20.048 66.569 1.000 36.16
ANISOU 1252 CG PRO 165 3341 6449 3948 -518 -349 -3
ATOM 1253 CD PRO 165 -4.197 19.816 65.734 1.000 35.70
                                                                                                                                                                                                           -518 -349 - 398
   ANISOU 1253 CD PRO 165 3440 6296 3828
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                              1254 N LEU 178 4.459 8.087 66.987 1.000 36.23
1254 N LEU 178 4509 3338 5918 -26 1216 1175
   ANISOU 1254 N
  ATOM 1255 CA LEU 178 4.994 9.117 66.116 1.000 28.63
ANISOU 1255 CA LEU 178 3397 3170 4312 377 1344 4 0 1
  ATOM 1256 CB LEU 178 5.882 8.534 65.027 1.000 30.08
ANISOU 1256 CB LEU 178 3497 3245 4688 760 752 -620
ANISOU 1256 CB LEU 178 3497 3245 4688 760 752 -620 ATOM 1257 CG LEU 178 3557 2950 4674 667 371 -979 ATOM 1258 CD1 LEU 178 7.859 7.367 64.073 1.000 32.13 ANISOU 1258 CD1 LEU 178 2972 4524 4713 586 810 -790 ATOM 1259 CD2 LEU 178 8.208 8.964 65.937 1.000 41.71 ANISOU 1259 CD2 LEU 178 5303 3695 6850 356 -1656 -1154 ATOM 1260 C LEU 178 2107 3534 4686 -175 1776 8 3 3 ATOM 1261 O LEU 178 2.845 9.351 65.086 1.000 39.60 ANISOU 1261 O LEU 178 2407 4624 8016 -1253 1290 2183 ATOM 1262 N ARG 179 2220 3437 4089 -216 878 74 1 ATOM 1263 CA ARG 179 3.231 11.973 64.321 1.000 25.04 ANISOU 1263 CA ARG 179 3.231 11.973 64.321 1.000 25.04 ANISOU 1264 C ARG 179 3.297 11.572 ATOM 1265 O ARG 179 2545 3242 5079 441 -332 -256 ATOM 1266 CB ARG 179 3.517 13.480 64.451 1.000 28.58 ANISOU 1266 CB ARG 179 3.517 13.480 64.451 1.000 28.58 ANISOU 1266 CB ARG 179 3.517 13.480 64.451 1.000 28.58 ANISOU 1266 CB ARG 179 3.980 317 3.600 26.00 27.000 28.58 ANISOU 1266 CB ARG 179 3.517 13.480 64.451 1.000 28.58 ANISOU 1266 CB ARG 179 3.500 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 317 3.600 31
                               1266 CB ARG 179 3980 3317 3561 -110 -843 5
1267 CG ARG 179 2.936 14.092 65.724 1.000 30.01
  ANISOU 1266 CB ARG 179 3980
                                                                                                                                                                                                            -110 -843 5 7
  ATOM
  ANISOU 1267 CG ARG 179 3817 3725 3862 57 -957 -37
ATOM 1268 CD ARG 179 3.307 15.570 65.757 1.000 31.51
                                                                                                                                                                                                            57 - 957 - 3.72
  ANISOU 1268 CD ARG 179 4457 3675 3840 90 -1514 - 33
ATOM 1269 NE ARG 179 2.925 16.126 67.058 1.000 37.82
                                                                                                                                                                                                            90 -1514 - 338
  ANISOU 1269 NE ARG 179 7035
                               1269 NE ARG 179 7035 3190 4144 153 -310 - 1270 CZ ARG 179 2.897 17.425 67.292 1.000 39.43
                                                                                                                                                                                                           153 -310 - 15
  ATOM
  ANISOU 1270 CZ ARG 179 8420 3029 3532 -479 580 4
ATOM 1271 NH1 ARG 179 3.213 18.286 66.331 1.000 59.73
                                                                                                                                                                                                            -479 580 400
ANISOU 1270 CZ ARG 1/9 8420 3029 3532 -4/9 880 4 0 ATOM 1271 NH1 ARG 179 3.213 18.286 66.331 1.000 59.73 ANISOU 1271 NH1 ARG 179 11745 4676 6273 -1045 3177 17 ATOM 1272 NH2 ARG 179 2.548 17.896 68.457 1.000 33.13 ANISOU 1272 NH2 ARG 179 5661 3832 3094 275 -1463 -ATOM 1273 N MET 180 4.455 11.099 62.424 1.000 21.43 ANISOU 1273 N MET 180 2013 2457 3674 -395 108 -2 ATOM 1274 CA MET 180 4.695 10.539 61.108 1.000 20.07 ANISOU 1274 CA MET 180 2346 1965 3315 -349 -3001 5 ATOM 1275 C MET 180 5.802 9.482 61.182 1.000 17.33 ANISOU 1275 C MET 180 2251 2080 2254 -332 -86 33 ATOM 1276 O MET 180 6.894 9.757 61.677 1.000 18.52 ANISOU 1276 O MET 180 2237 2019 2781 -398 -79 5 ATOM 1277 CB MET 180 2237 2019 2781 -398 -79 5 ATOM 1277 CB MET 180 2571 2321 3709 -197 -549 68 ATOM 1278 CG MET 180 3918 3095 3588 -453 -654 91 ATOM 1278 CG MET 180 3918 3095 3588 -453 -654 91 ATOM 1279 SD MET 180 2936 2942 3626 -399 124 8 5 ATOM 1280 CE MET 180 2936 ATOM 1280 CE MET 180 2936 ATOM 1280 CE MET 180 5917 3450 4690 -258 -2680 1 ATOM 1281 N ALA 181 5.467 8.295 60.680 1.000 16.99 ANISOU 1281 N ALA 181 5.467 8.295 60.680 1.000 16.99 ANISOU 1281 N ALA 181 5.467 8.295 60.680 1.000 16.99 ANISOU 1281 N ALA 181 2144 2139 2174 -90 -558 25
                                                                                                                                                                                                            -1045 3177 1722
                                                                                                                                                                                                                              -1463 -173
                                                                                                                                                                                                            -395 108 -222
                                                                                                                                                                                                            -349 -300 1 5 1
                                                                                                                                                                                                            -332 -86 337
                                                                                                                                                                                                            -197 -549 683
                                                                                                                                                                                                             -453 -654 9 1 3
                                                                                                                                                                                                             -399 124 851
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- 132 -
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ANISOU 1282 CA ALA 181 2275
ATOM 1283 CB ALA 181 5.668
ANISOU 1283 CB ALA 181 2857
ATOM 1284 C ALA 181 7.576
ANISOU 1284 C ALA 181 2223
ATOM 1285 O ALA 181 7.458
ANISOU 1285 O ALA 181 2268
ATOM 1286 N PRO 182 8.698
ANISOU 1286 N PRO 182 8.698
ANISOU 1287 CD PRO 182 8.983
ANISOU 1288 CA PRO 182 9.865
ANISOU 1288 CA PRO 182 2573
                                                       1282 CA ALA 181 6.396 7.168 60.676 1.000 16.12
                   ATOM
      1288 CA PRO 182 2573 1336 1706 -101 -86 2 9 9 1289 CB PRO 182 2570 1289 59.649 1.000 16.20
                                                                                        TYR 184 10.849 7.907 53.215 1.000 10.61
TYR 184 1453 1027 1552 -41 -380 1 1
TYR 184 11.483 8.800 52.256 1.000 11.36
TYR 184 1475 1104 1738 -71 -264 1 7
TYR 184 12.628 8.151 51.481 1.000 11.79
TYR 184 1631 1114 1734 -62 -197 3 6
TYR 184 12.368 6.907 50.677 1.000 11.29
TYR 184 1680 921 1688 225 -893 1 7 4
ATOM 1304 CA
ANISOU 1304 CA TYR 184 12.628
ATOM 1305 CB TYR 184 12.628
ANISOU 1305 CB TYR 184 1631 1114 1734
ATOM 1306 CG TYR 184 12.368 6.907 50.677 1.000 11.2
ANISOU 1306 CG TYR 184 1680 921 1688 225 -893 1 7 4
ANISOU 1307 CD1 TYR 184 12.156 5.659 51.268 1.000 11.76
ATOM 1308 CE1 TYR 184 11.911 4.526 50.492 1.000 12.64
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ATOM 1309 CD2 TYR 184 1252 1302 1674 109 -283 9
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ANISOU 1310 CE2 TYR 184 1944 1422 1546 49 -384 7 3
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ATOM 1311 CZ TYR 184 1717 1304 1972 30 -611 6 7
TYR 184 1717 1304 1972 30 -611 6 7
                                                                                                                                                                                                                                                                    -41 -380 1 1 0
         ATOM 1304 CA
ANISOU 1304 CA
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- 133 -ANISOU 1312 OH TYR 184 2028 1471 2373 42 -476 - 247 TYR 184 10.447 9.390 51.314 1.000 11.50 1313 C 1709 -18/ -201 51.089 1.000 11.75 -106 -171 4 ANISOU 1313 C TYR 184 1445 1215 -187 -201 3 4 8 TYR 184 9.362 ATOM 1314 0 8.797 ANISOU 1314 O TYR 184 1305 1308 -106 -171 4 2 7 1315 N ASP 185 10.784 10.557 50.743 1.000 10.79 ATOM ANISOU 1315 N ASP 185 1581 1069 1449 -141 -132 1 1 8 1316 CA ATOM ASP 185 9.861 11.218 49.815 1.000 9.10 ANISOU 1316 CA ASP 185 1089 1093 1277 -326 23 2 0 6 185 9.934 12.743 49.886 1.000 10.13 1317 CB ASP ANISOU 1317 CB ASP 185 1427 1095 1327 -298 -178 1 7 7 1318 CG ASP 185 9.540 13.388 51.185 1.000 11.79 ATOM ANISOU 1318 CG ASP 185 1797 1350 1333 -250 -149 1 1 1319 OD1 ASP ATOM 185 9.681 14.638 51.278 1.000 13.79 185 2050 1316 1875 135 -52 -185 9.114 12.755 52.189 1.000 13.31 ANISOU 1319 OD1 ASP 135 -52 - 26 1320 OD2 ASP

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 9.114
 12.755
 52.189
 1.000
 13.31

 185
 1805
 1848
 1405
 -411
 -63
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 9.44

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 1036
 1150
 1401
 -309
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 SER
 187
 1427
 1191
 1370
 195
 -107
 4

 SER
 187
 9.221
 15.103
 46.002
 1.000
 10.56

 SER
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 1048
 1857
 298
 161
 5

 SER
 187
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 46.726
 1.000
 13.01

 SER
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 1343
 1432
 2169
 -132
 -295
 2

 SER
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 14.062
 44.336
 1.000
 10.47
 3

 SER
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 1447
 862
 1669
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 -3
 145
 3

 SER
 187
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 13.246
 44.513
 1.000
 10.54
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 SER
 187
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 -91
 -7
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 978
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 4

 MET
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 1441
 182
 58
 3
 7

 195 -107 4 8 8 ATOM 1333 CB ANISOU 1333 CB 161 532 1334 OG ANISOU 1334 OG -132 -295 2 0 1 ATOM 1335 C ANISOU 1335 C MOTA 1336 0 ANISOU 1336 O 1337 N ATOM ANISOU 1337 N MOTA 1338 CA ANISOU 1338 CA 188 1394 MET 942 1441 182 58 3 7 ATOM 1339 CB MET ANISOU 1339 CB MET 1340 CG ATOM MET ANISOU 1340 CG MET 188 1403 1172 1756 46 -51 2 1 4 ATOM 1341 SD MET 188 14.687 16.134 40.891 1.000 12.71 ANISOU 1341 SD 188 1619 1272 1940 139 137 1 9 8 188 16.061 17.267 40.790 1.000 13.86 MET 1342 CE MET ANISOU 1342 CE 188 1862 MET 1399 2003 -2 911 - 9 0

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ANISOU 1343 C MET 188 1325 1586 1698 169 -18 -28
ATOM 1344 C MET 188 13.971 15.727 44.804 1.000 11.52
ANISOU 1344 O MET 188 1288 1553 1535 144 132 8 7
ATOM 1345 N VAL 189 12.362 17.290 44.838 1.000 10.00
ANISOU 1345 N VAL 189 12.90 1217 1292 53 -175 6
ATOM 1346 CA VAL 189 12.745 17.894 46.099 1.000 9.70
ANISOU 1346 CA VAL 189 12.09 1057 1420 -212 -45 -1 9
ATOM 1347 CB VAL 189 13.618 19.154 45.979 1.000 9.97
ANISOU 1347 CB VAL 189 13.618 19.154 45.979 1.000 9.97
ANISOU 1347 CB VAL 189 1288 1103 1398 -238 129 18 9
ATOM 1348 CG1 VAL 189 1288 1103 1398 -238 129 18 9
ANISOU 1348 CG1 VAL 189 14.953 18.837 45.266 1.000 13.45
ANISOU 1348 CG1 VAL 189 1334 1410 2368 -236 390 14 3
ATOM 1349 CG2 VAL 189 12.899 20.289 45.264 1.000 12.24
ANISOU 1349 CG2 VAL 189 1715 1242 1693 -25 150 29 5
ATOM 1350 C VAL 189 1715 1242 1693 -25 150 29 5
ATOM 1350 C VAL 189 10.405 18.245 46.871 1.000 10.10
ATOM 1351 O VAL 189 10.405 18.399 46.250 1.000 9.53
                                                                                                                      - 134 -
                                                                                                                                                                          169 -18 -285
                                                                                                                                                                          -212 -45 -19
                                                                                                                                                                          -238 129 189
                                                                                                                                                                          -236 390 143
                                                                                                                                                                                          150 295
                                                         VAL 189 1089 1600 1149 -456 -156 - VAL 189 10.405 18.399 46.250 1.000 9.53
                                                                                                                                                                         -456 -156 - 73
                           1351 O VAL 189 1153 1249 1217 -222 -190 8
1352 N THR 190 11.609 18.327 48.187 1.000 8.66
1352 N THR 190 1273 894 1123 15 -202 127
1353 CA THR 190 10.565 18.771 49.091 1.000 9.64
    ANISOU 1351 O
                                                                                                                                                                        -222 -190 8
    ATOM
                       1352 N
ANISOU 1352 N
  ANISOU 1371 CG1 ILE 192 2633 1658 1601 -400 -48 -1 ATOM 1372 CD1 ILE 192 9.845 18.765 55.339 1.000 25.71 ANISOU 1372 CD1 ILE 192 5869 1608 2290 -175 -1566 - ATOM 1373 C ILE 192 9.966 23.809 55.253 1.000 11.47
                                                                                                                                                                         -400 -48 -175
                                                                                                                                                                         -175 -1566 -301
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- 135 -ANISOU 1373 C ILE 192 1330 1427 -4 -222 -122 1603 ILE 192 11.123 24.106 55.567 1.000 13.33 1374 0 ANISOU 1374 O ILE 192 1344 1738 1981 -96 -289 - 2 24.525 55.602 1.000 15.78 -289 - 219 1375 N GLN 193 8.904 ANISOU 1375 N GLN 193 1316 2462 2219 -64 -5 -975 1376 CA GLN 25.653 56.533 1.000 14.56 193 8.987 ANISOU 1376 CA GLN 193 1582 1858 2091 212 -304 -5291377 CB GLN 193 8.449 ATOM 26.975 56.020 1.000 20.03 ANISOU 1377 CB GLN193 2226 2203 3180 318 -329 1 4 2 GLN 193 9.203 1378 CG 27.684 54.914 1.000 23.86 MOTA ANISOU 1378 CG GLN 193 3399 2492 313 45 28 0 3174 GLN 193 8.665 29.079 54.675 1.000 22.92 ATOM 1379 CD ANISOU 1379 CD GLN 193 3250 2363 3097 78 -477 205 1380 OE1 GLN 193 7.603 ATOM 29.292 54.099 1.000 27.68 ANISOU 1380 OE1 GLN 193 4175 3310 3031 552 -1214 2 91381 NE2 GLN 193 9.411 ATOM 30.075 55.134 1.000 27.01 ANISOU 1381 NE2 GLN 193 3187 2667 4408 -440 124 1 7 GLN 193 8.216 ATOM 1382 C 25.265 57.804 1.000 15.14 ANISOU 1382 C GLN 193 1945 1827 1982 136 -174 - 722MOTA 1383 0 GLN 193 7.147 24.662 57.714 1.000 27.80 ANISOU 1383 O GLN 193 2523 6225 1817 -1586 -592 2 3 5 194 8.714 194 2994 194 8.100 MOTA 1384 N GLN 25.552 58.978 1.000 19.80 ANISOU 1384 N GLN 2502 2025 -632 -752 3 3 ATOM 1385 CA GLN25.080 60.213 1.000 22.89 ANISOU 1385 CA GLN 194 3961 194 7.763 2626 2110 493 -20 5 2 MOTA 1386 C GLN 26.236 61.141 1.000 27.79 ANISOU 1386 C GLN194 4886 2757 2916 823 25 - 262 MOTA 1387 O 194 8.424 194 4727 GLN 27.258 60.983 1.000 30.03 ANISOU 1387 O GLN 3168 3516 368 -259 - 910ATOM 1388 CB GLN194 9.086 24.170 60.950 1.000 23.97 194 3952 ANISOU 1388 CB ${\tt GLN}$ 3133 2021 846 483 352 1389 CG ${ t GLN}$ 194 9.398 22.835 60.314 1.000 21.94 ANISOU 1389 CG GLN 194 2740 3238 2358 683 -182 - 101390 CD 194 10.546 GLN22.148 61.052 1.000 20.51 ANISOU 1390 CD GLN194 2450 3433 1911 509 -321 - 4291391 OE1 GLN MOTA 194 11.707 22.142 60.627 1.000 20.80 ANISOU 1391 OE1 GLN 194 2245 2996 2662 -171 -382 -681ATOM 1392 NE2 GLN 194 10.223 21.585 62.197 1.000 24.91 ANISOU 1392 NE2 GLN 194 2539 3902 3023 210 -365 7 6 0 ATOM 1393 N THR 195 6.817 26.035 62.030 1.000 32.47 ANISOU 1393 N THR 195 5716 2729 3891 1095 1056 - 616 ATOM 1394 CA THR 195 6.588 26.708 63.282 1.000 35.83 ANISOU 1394 CA THR 195 6329 3539 3748 1011 999 - 722 ATOM 1395 CB THR 195 5.263 27.492 63.357 1.000 37.96 ANISOU 1395 CB THR 195 5756 4304 4365 647 2095 - 1151 ATOM 1396 OG1 THR 195 4.191 26.576 63.604 1.000 48.36 ANISOU 1396 OG1 THR 195 6874 6076 5423 -806 2581 -1842 1397 CG2 THR 195 4.958 ATOM 28.175 62.033 1.000 44.54 ANISOU 1397 CG2 THR 195 2944 7471 6510 -872 -963 6 2 1 ATOM 1398 C THR 195 6.590 25.684 64.429 1.000 48.86 ANISOU 1398 C THR 195 10133 4924 3508 -321 -1356 -221 ATOM 1399 0 THR 195 6.122 24.544 64.293 1.000 64.12 ANISOU 1399 O THR 195 13267 4150 6945 -264 -4541 1682 1400 N MOTA PHE 201 12.035 21.374 72.205 1.000 71.12 ANISOU 1400 N PHE 201 13961 9034 4028 -5932 -1658 -1741 ATOM 1401 CA 201 11.775 201 7918 PHE 20.053 71.629 1.000 49.44 ANISOU 1401 CA PHE 7543 3326 -3128 1317 -1488 MOTA 1402 CB 201 10.469 PHE 19.464 72.181 1.000 47.85 ANISOU 1402 CB PHE 201 7119 6892 4168 -1869 1937 - 1899 ATOM 1403 CG PHE 201 10.130 18.113 71.545 1.000 46.41 ANISOU 1403 CG PHE 201 6643 6596 4396 -2038 1879 - 1497

- 136 -1404 CD1 PHE 201 10.738 16.954 71.991 1.000 50.03 ATOM ATOM 1404 CD1 FHE 201 7982 6634 ATOM 1405 CD2 PHE 201 9.220 18.00 4393 -2326 1092 - 991 18.001 70.513 1.000 42.63 ANISOU 1405 CD2 PHE 201 5458 6427 4313 -1097 2449 -2 ATOM 1406 CE1 PHE 201 10.434 15.739 71.417 1.000 49.95 -1097 2449 - 2268 ANISOU 1406 CE1 PHE 201 8275 6464 4240 -2047 227 ATOM 1407 CE2 PHE 201 8.901 16.783 69.934 1.000 41.38
ANISOU 1407 CE2 PHE 201 6016 5946 3762 -578 2006 --2047 227 - 716 PHE 201 6016 5946 3762 -578 2006 - PHE 201 9.515 15.636 70.392 1.000 44.74 -578 2006 - 1844 ANISOU 1408 CZ PHE 201 7075 201 7075 6261 3663 -1063 1020 -201 11.722 20.110 70.107 1.000 42.42 6261 -1063 1020 - 975 1409 C ATOM PHE ANISOU 1410 O PHE 201 6324 6442 3351 -1964 717 -14
ANISOU 1410 O PHE 201 11.007 20.941 69.536 1.000 47.79
ATOM 1411 N VAL 202 12.477 19.232 69.449 1.000 34.04
ATOM 1411 N VAL 202 4525 5852 2558 -1948 7 -425
ANISOU 1412 CA VAL 202 12.535 19.245 67.993 1.000 25.09
ATOM 1413 CB VAL 202 3221 3752 2558 -1041 -182 9 9
ANISOU 1413 CB VAL 202 2832 3430 2432 -577 -691 -19 ANISOU 1409 C -1964 717 -1441 -762 691 -2416 1413 CB VAL 202 2832 3430 2432 -577 -691 -1
1414 CG1 VAL 202 14.053 19.387 65.965 1.000 26.02 -577 -691 -198 ANISOU 1414 CG1 VAL 202 3821 3594 2470 -958 35 - 277 1415 CG2 VAL 202 14.771 20.443 68.078 1.000 24.69 ATOM ANISOU 1415 CG2 VAL 202 3043 3473 2867 -786 - 410 - 320ATOM 1416 C VAL 202 11.798 18.035 67.421 1.000 20.69 ANISOU 1416 C VAL 202 3027 2810 2023 VAL 202 12.288 16.914 67.581 1.000 26.08 VAL 202 3294 3219 3396 -136 452 8 SER 203 10.662 18.234 66.766 1.000 20.21 SER 203 9.820 17.192 66.218 1.000 20.37 SER 203 3149 2709 1884 -355 129 -2 -648 58 6 1 5 ATOM 1417 0 ANISOU 1417 O -136 452 884 ATOM 1418 N ANISOU 1418 N -414 25 - 152 1419 CA ATOM ANISOU 1419 CA 203 3149 2709 1884 -355 129 -256 ATOM 203 8.437 17.779 65.896 1.000 24.72 1420 CB SER ANISOU 1420 CB 203 2726 4106 2558 -178 369 -203 7.841 18.239 67.097 1.000 31.80 SER 369 -1015 ATOM 1421 OG SER ANISOU 1421 OG SER 203 3328 5782 2974 -457 1175 -203 10.367 16.524 64.958 1.000 19.13 -457 1175 -1104 1422 C ATOM SER ANISOU 1422 C SER 203 2580 2647 2040 203 2580 2647 2040 -339 170 -203 10.279 15.302 64.832 1.000 17.01 -339 170 -244 ATOM 1423 0 SER ANISOU 1423 O 203 2311 SER 203 2311 2625 1527 -414 206 -204 10.902 17.259 63.998 1.000 16.16 -414 206 - 18 ATOM 1424 N LEU ANISOU 1424 N LEU 204 2142 1976 2024 71 77 - 292 LEU 204 11.403 16.679 62.740 1.000 14.07 ATOM ATOM 1425 CA ANISOU 1425 CA LEU 204 1670 1626 2049 -22 -24 -: LEU 204 11.269 17.704 61.618 1.000 13.80 LEU 204 1670 -22 -24 -283 ATOM 1426 CB ANISOU 1426 CB LEU 204 1549 1763 204 11.647 17.272 60.212 1.000 14.13 1931 -249 -340 -2771427 CG ATOM LEU ANISOU 1427 CG LEU 204 1726 1722 1919 -253 -482 -412 1428 CD1 LEU 204 10.770 16.134 59.680 1.000 18.76 ANISOU 1428 CD1 LEU 204 2579 2895 1654 -1297 -927 - 106 1429 CD2 LEU ATOM 204 11.609 18.478 59.255 1.000 16.20 ANISOU 1429 CD2 LEU 204 1987 2095 2074 65 75 - 123 ATOM 1430 C 204 12.832 16.140 62.885 1.000 14.81 LEU ANISOU 1430 C LEU 204 1734 1748 2144 9 -199 -250 204 13.699 16.853 63.397 1.000 15.52 204 1734 1431 0 ATOM LEU ANISOU 1431 O LEU 204 1833 1789 2274 -59 -435 - 42 GLN 205 13.065 14.900 62.469 1.000 14.42 GLN 205 1847 1804 1827 189 -120 - GLN 205 14.288 14.143 62.574 1.000 12.76 GLN 205 1777 1655 1419 43 -347 -11 GLN 205 14.622 13.434 61.260 1.000 11.12 1432 N ATOM ANISOU 1432 N 189 -120 - 153 1433 CA GLNANISOU 1433 CA 43 - 347 - 113 1434 C

ANISOU 1434 C GLN 205 1412 1474 1338 49 -468 -21 ATOM 1435 O GLN 205 13.707 12.927 60.606 1.000 13.97 ANISOU 1435 O GLN 205 1622 2235 1449 -293 -449 -147 ATOM 1436 CB GLN 205 14.164 13.062 63.662 1.000 15.57 ANISOU 1437 CG GLN 205 13.863 13.635 65.032 1.000 18.58 ATOM 1438 CD GLN 205 3321 2286 1451 689 -129 8 2 ATOM 1438 CD GLN 205 3321 2286 1451 689 -129 8 2 ATOM 1438 CD GLN 205 3321 2286 1451 689 -129 8 2 ATOM 1438 CD GLN 205 3587 3465 2091 520 -499 -570 ANISOU 1439 OE1 GLN 205 3587 3465 2091 520 -499 -570 ANISOU 1439 OE1 GLN 205 3550 3464 4251 14 -270 -1800 ANISOU 1440 NE2 GLN 205 3550 3464 4251 14 -270 -1800 ANISOU 1440 NE2 GLN 205 3550 3464 4251 14 -270 -1800 ANISOU 1440 NE2 GLN 205 3550 3464 4251 14 -270 -1800 ANISOU 1440 NE2 GLN 205 3550 3464 4251 14 -270 -1800 ANISOU 1440 NE2 GLN 205 3550 3464 4251 14 -270 -1800 ANISOU 1440 NE2 GLN 205 3550 3464 4251 14 -270 -1800 ANISOU 1440 NE2 GLN 205 3550 3464 4251 14 -270 -1800 ANISOU 1440 NE2 GLN 205 3550 3464 59.731 1.000 23.01 ANISOU 1441 N ALA 206 15.893 13.401 60.893 1.000 12.63 ANISOU 1441 N ALA 206 15.893 13.401 60.893 1.000 12.63 ANISOU 1442 CA ALA 206 16.335 12.649 59.731 1.000 13.77 ANISOU 1442 CA ALA 206 16.693 13.519 58.528 1.000 16.34 ANISOU 1444 C ALA 206 16.693 13.519 58.528 1.000 16.34 ANISOU 1444 C ALA 206 17.567 11.813 60.046 1.000 15.92 ANISOU 1444 C ALA 206 17.567 11.813 60.046 1.000 15.92 ANISOU 1444 C ALA 206 17.567 11.813 60.046 1.000 15.92 ANISOU 1444 C ALA 206 1877 1772 2377 150 -356 3 0 ANISOU 1445 O ALA 206 1877 1772 2377 150 -356 3 0 ANISOU 1445 O ALA 206 1877 1772 2377 150 -356 3 0 ANISOU 1446 N GLU 207 17.707 10.712 59.305 1.000 16.98 ANISOU 1446 N GLU 207 17.707 10.712 59.305 1.000 16.98 ANISOU 1446 N GLU 207 17.707 10.712 59.305 1.000 16.98 ANISOU 1446 N GLU 207 17.707 10.712 59.305 1.000 16.98 ANISOU 1446 N GLU 207 17.707 10.712 59.305 1.000 16.98 ANISOU 1446 N GLU 207 17.707 10.712 59.305 1.000 16.98 ANISOU 1446 N GLU 207 17.707 10.712 59.305 1.000 16.98 ANISOU 1446 N GLU 207 1981 - 137 --603 123 -277 U 1445 O ALA 206 1877 1772 2377 150 -356 3 1446 N GLU 207 17.707 10.712 59.305 1.000 16.98 U 1446 N GLU 207 1981 2086 2383 -335 348 -1 1447 CA GLU 207 18.938 9.942 59.364 1.000 20.58 U 1447 CA GLU 207 2198 1938 3684 -164 490 -1 ANISOU 1446 N -335 348 -186 ATION 1447 CA GLU 207 18.938 9.942 59.364 1.000 20.58 ANISOU 1447 CA GLU 207 2198 1938 3684 -164 490 -1 0 ATOM 1448 C GLU 207 2198 1938 3684 -164 490 -1 0 ATOM 1448 C GLU 207 19.848 2037 3260 272 185 5 5 8 ATOM 1449 O GLU 207 19.848 2037 3260 272 185 5 5 8 ATOM 1449 O GLU 207 1746 2145 3034 52 8 -45 ATOM 1450 CB GLU 207 18.665 8.612 58.676 1.000 25.81 ANISOU 1450 CB GLU 207 19.879 7.737 58.429 1.000 30.08 ANISOU 1451 CG GLU 207 19.879 7.737 58.429 1.000 30.08 ANISOU 1451 CG GLU 207 19.429 6.356 57.959 1.000 30.08 ANISOU 1452 CD GLU 207 19.429 6.356 57.959 1.000 29.93 ATOM 1453 OE1 GLU 207 5549 2024 3798 1179 -2099 -123 ANISOU 1454 OE2 GLU 207 19.491 5.471 58.839 1.000 35.14 ANISOU 1454 OE2 GLU 207 782 2692 4879 938 -931 8 5 ATOM 1455 N VAL 208 21.146 10.997 59.414 1.000 16.97 ANISOU 1455 N VAL 208 21.146 10.997 59.414 1.000 16.97 ANISOU 1455 CA VAL 208 22.376 11.593 58.902 1.000 37.77 ANISOU 1456 CA VAL 208 22.376 11.593 58.902 1.000 17.77 ANISOU 1458 CG1 VAL 208 22.376 11.593 58.902 1.000 16.97 ANISOU 1458 CG1 VAL 208 22.355 13.68 58.40 1.000 20.76 ANISOU 1458 CG1 VAL 208 22.455 13.68 58.40 1.29 33 50 41 1 1.000 16.89 ANISOU 1458 CG1 VAL 208 23.555 13.68 58.40 1.29 256 -423 647 14 8 ANISOU 1460 C VAL 208 23.555 13.68 58.40 1.000 20.74 ANISOU 1460 C VAL 208 23.555 13.68 58.40 1.000 20.74 ANISOU 1460 C VAL 208 23.555 13.68 58.40 1.000 20.74 ANISOU 1460 C VAL 208 23.555 13.68 58.40 1.000 20.74 ANISOU 1460 C VAL 208 23.555 13.68 58.40 1.000 20.74 ANISOU 1460 C VAL 208 23.555 13.68 58.40 1.000 20.74 ANISOU 1461 O VAL 208 23.555 13.68 58.40 1.000 20.74 ANISOU 1461 O VAL 208 23.555 3217 1.58 13.2 ANISOU 1461 O VAL 208 23.555 3217 1.58 13.2 ANISOU 1461 O VAL 208 23.555 3217 1.58 13.2 ANISOU 1461 O VAL 208 23.555 3217 1.58 13.2 ANISOU 1461 O VAL 208 23.555 3217 1.58 13.2 ANISOU 1461 O VAL 208 23.555 3217 1.58 13.2 ANISOU 1461 O VAL 208 23.555 3217 1.58 13.2 ANISOU 1461 O VAL 208 23.555 3217 1.58 13.2 ANISOU 1461 O VAL 208 23.555 3217 1.58 13.2 ANISOU 1461 O VAL 208 23.555 3217 1.58 12.000 20.74 ANISOU 1461 O VAL 208 23 ATOM ANISOU 1447 CA GLU 207 2198 3684 -164 490 - 10ANISOU 1463 CA GLY 209 2171 3040 3910 549 -396 709 ATOM 1464 C GLY 209 25.123 8.364 60.082 1.000 25.00 ANISOU 1464 C GLY 209 2874 3156 3470 1406 772 649

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- 138 -
           1465 0
                      GLY 209 25.850 7.934
                                                     60.991 1.000 35.98
  ANISOU 1465 O
                      GLY 209 4448
                                            3946
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                                                               1425 -426 1769
  ATOM
           1466 N
                      GLY 210 23.951
                                           7.786
                                                     59.869 1.000 25.89
  ANISOU 1466 N
                      GLY
                           210 3802
                                           2756
                                                     3278
                                                               523
                                                                      899 749
  ATOM
           1467 CA
                      GLY
                            210 23.477 6.678
                                                     60.671 1.000 26.43
  ANISOU 1467 CA
                      GLY
                            210 4479
                                           2136
                                                     3427
                                                              1228 742 912
  ATOM
           1468 C
                      GLY
                            210 22.885 7.025
                                                     62.016 1.000 28.45
  ANISOU 1468 C
                      GLY
                            210 5472 2099
                                                     3237
                                                              831 1029 1175
  ATOM
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           1469 0
                      GLY
  ANISOU 1469 O
                      GLY
                            210 7322 2719
                                                     5256
                                                               1881 2759 2360
  ATOM
          1470 N
                           211 22.651 8.281 62.338 1.000 25.78
                      ALA
                           211 4671 2359
  ANISOU 1470 N
                            211 4671 2359 2763 1370 724 1197
211 22.048 8.671 63.613 1.000 23.74
                      ALA
          1471 CA ALA
  ANISOU 1471 CA ALA 211 2966 3156

    211
    2966
    3156
    2896
    727
    339
    663

    211
    23.093
    9.333
    64.496
    1.000
    29.57

  MOTA
          1472 CB
                    ALA
 ATOM 1472 CB ALA 211 235.093 5.333 04.490 1.000 29.37 ANISOU 1472 CB ALA 211 2957 4372 3906 834 -96 6 ANISOU 1473 C ALA 211 20.900 9.626 63.360 1.000 21.19 ATOM 1474 O ALA 211 3090 2611 2350 484 178 7 ATOM 1474 O ALA 211 20.936 10.381 62.399 1.000 23.91
                                                              834 -96 6 9
                                                                      178 741
                          211 3771
                                           2659
                                                    2653
                                                              -30
                                                                    -66 930
  ATOM
          1475 N
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                    PHE
                                                   64.204 1.000 19.88
 ANISOU 1475 N
                    PHE
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                                           2577
                                                     2375
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                                                                      -128 3 7 4
 ATOM
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          1476 CA PHE
 ANISOU 1476 CA PHE
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                                           2257
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                                                              284
                                                                     -565 3 1 7
 ATOM
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                     PHE
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 ANISOU 1477 C
                     PHE
                          212 3004 2480
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                          212 19.893 12.230 65.569 1.000 21.10
212 2497 3558 1964 -381 406
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                                                                     -640 6 8
 ATOM
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 ANISOU 1478 O
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          1479 CB
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 ANISOU 1479 CB
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                          212 17.010 8.950 64.912 1.000 23.45
212 2161 3496 3253 -376 -282 -
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                                                                     -197 - 184
 ATOM
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 ANISOU 1480 CG
                    PHE
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          1481 CD1 PHE
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212 2545 3115 3206 -382 -350 -
212 17.029 8.302 63.687 1.000 25.83
 ATOM
 ANISOU 1481 CD1 PHE
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 ATOM
          1482 CD2 PHE
 ANISOU 1482 CD2 PHE
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 ATOM
 ANISOU 1483 CE1 PHE 212 3784
         1483 CE1 PHE 212 3784 3544 3362 -1119 96 -97 1484 CE2 PHE 212 16.419 7.072 63.569 1.000 23.04 1484 CE2 PHE 212 2504 2960 3289 382 -232 -5 1485 CZ PHE 212 15.781 6.486 64.651 1.000 27.88
                                                             -1119 96 - 973
 ATOM
 ANISOU 1484 CE2 PHE 212 2504
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 ATOM
                   PHE 212 15.781 5.485 64.551 1.000 27.00
PHE 212 3658 3977 2957 -1072 -501 -
THR 213 19.076 12.936 63.578 1.000 18.30
THR 213 2690 2083 2181 149 -583 -
THR 213 19.566 14.310 63.681 1.000 17.99
THR 213 1976 2139 2721 230 -686 -2
THR 213 20.515 14.586 62.498 1.000 20.43
THR 213 1798 2280 3683 140 -119 -4
THR 213 21.638 13.695 62.629 1.000 25.33
 ANISOU 1485 CZ
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· ATOM
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 ANISOU 1486 N
                                                                   -583 - 93
         1487 CA
 ATOM
 ANISOU 1487 CA
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         1488 CB
 ANISOU 1488 CB
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         1489 OG1 THR
 ANISOU 1489 OG1 THR
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                                                    3676
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         1490 CG2 THR
                                                                     71 5 2 8
 ATOM
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ANISOU 1490 CG2 THR
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 ATOM
         1491 C
                          213 18.391 15.277 63.641 1.000 15.53
                     THR
ANISOU 1491 C
                          213 1732 2135 2032 111 -557 -1
213 17.533 15.195 62.761 1.000 16.11
                     THR
                          213 1732
                                                              111 -557 - 167
 ATOM
         1492 0
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ANISOU 1492 O
                          213 1742
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                                                    2180
                                                              -327 -669 5 6
         1493 N
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                     ASP
ANISOU 1493 N
                     ASP
                           214 2025
                                          2046
                                                    1857
                                                              64 - 405 2
         1494 CA
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                    ASP
ANISOU 1494 CA
                    ASP
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                                          1722 2072
                                                              2 -1010 - 242
ATOM
         1495 CB
                          214 17.744 18.200 65.822 1.000 17.13
                    ASP
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					- 139 -		
ANISOU			ASP	214 2528	1893	2086	-226 -1022 -247
ATOM ANISOU	1496		ASP ASP	214 17.612 214 3138	17.672	67.219	1.000 20.21
ATOM	1497			214 3138 214 17.079	2495 16.571	2045 67.460	-451 -1276 -148 1.000 20.87
ANISOU	1497	OD1	ASP	214 2778	2632	2518	-247 -505 1 5 1
ATOM	1498			214 18.076	18.401	68.127	1.000 28.05
ANISOU				214 5110	3118	2429	-257 -1997 -619
ATOM ANISOU	1499		ASP ASP	214 17.314 214 2029	18.146	63.441	1.000 15.14
ATOM	1500		ASP	214 2029	1822 18.552	1901 62.897	182 -574 - 319 1.000 17.63
ANISOU	1500	0	ASP	214 1956	2032	2710	-214 -810 - 15
ATOM	1501		LEU	215 16.105	18.493	63.027	1.000 14.69
ANISOU ATOM	1501		LEU LEU	215 1936	1758	1887	38 -334 242
ANISOU			LEU	215 15.915 215 1820	19.504 1753	61.979 1498	1.000 13.35 89 -22 5 9
MOTA	1503	СВ	LEU	215 15.352	18.819	60.734	1.000 14.24
ANISOU			LEU	215 1735	2167	1506	-98 75 - 3
ATOM ANISOU	1504		LEU	215 16.291	17.813	60.056	1.000 16.39
ATOM	1505		LEU	215 2031 215 15.517	2285 16.999	1911	-340 320 -424
ANISOU	1505	CD1	LEU	215 3139	2024	59.031 3427	1.000 22.61 -10 -801 -877
ATOM	1506	CD2	LEU	215 17.482	18.543	59.434	1.000 26.93
ANISOU ATOM	1506 1507	CD2		215 1998	5409	2827	-1083 909 -542
ANISOU			LEU LEU	215 15.002 215 1770	20.622	62.500	1.000 14.65
ATOM	1508	0	LEU	215 1770	1607 20.662	2190 62.151	86 -165 - 95 1.000 19.45
ANISOU			LEU	215 1748	2165	3476	116 -303 - 203
ATOM ANISOU	1509		PRO	216 15.552	21.523	63.314	1.000 15.99
ANISOU	1510		PRO PRO	216 2390 216 16.955	1970	1715	-164 21 -175
ANISOU			PRO	216 2900	21.601 2306	63.757 2155	1.000 19.37 -83 -790 -548
ATOM	1511		PRO	216 14.760	22.620	63.846	1.000 18.68
ANISOU			PRO	216 3104	2017	1976	12 -74 - 420
ATOM ANISOU		CB	PRO PRO	216 15.649 216 3592	23.227	64.949	1.000 18.63
ATOM	1513		PRO	216 3392	1517 22.847	1971 64.581	-120 -421 9 1.000 22.35
ANISOU	1513	CG	PRO	216 3401	2426	2666	-419 -427 - 783
ATOM	1514		PRO	216 14.461	23.700	62.819	1.000 18.50
ANISCU ATOM	1514		PRO PRO	216 2921 216 15.024	2083	2026	58 - 465 - 473
ANISOU			PRO	216 2752	23.854 2453	61.731 2325	1.000 19.82 -32 -375 1 9
ATOM .			TYR	217 13.487		63.194	1.000 20.05
ANISOU			TYR	217 3213	1981	2422	90 -482 -718
ATOM ANISOU	1517	CA	\mathtt{TYR}	217 13.178 217 2849	25.662	62.308	1.000 22.97
ATOM		C	TYR	217 2849 217 14.347	2652 26.647	3227 62.283	211 -1467 - 313 1.000 23.92
ANISOU	1518	С	TYR	217 4139	2131	2819	-337 -1776 -165
ATOM	1519	0	TYR	217 15.149	26.726	63.213	1.000 30.46
ANISOU ATOM	1520		TYR TYR	217 4321	3440	3812	-1118 -2477 7 2 8
ANISOU	1520	CB	TYR	217 11.891 217 3958	26.314 3294	62.768 5164	1.000 32.68 1148 -874 - 783
ATOM	1521	CG	TYR	217 12.064	27.462	63.718	1.000 44.77
ANISOU			TYR	217 6829	4326	5854	895 38 - 1870
ATOM ANISOU			TYR TYR	217 11.853 217 10311	28.763	63.285	1.000 54.26
MOTA	1523	CD2	TYR	217 10311 217 12.428	3688 27.243	6615 65.043	-323 132 -1945 1.000 57.77
ANISOU	1523	CD2	TYR	217 10635	5155	6158	-1027 -1446 -1931
ATOM	1524	CE1	TYR	217 12.011	29.816	64.174	1.000 60.33
ANISOU ATOM	1524	CEI	$\Delta A B$	217 11807 217 12.585	4345	6772	-1101 -132 -2259
ANISOU	1525	CE2	TYR	217 12.585	28.296 5199	65.926 6832	1.000 64.51 -1936 -1520 -2074
				· - -			

	- 140 -
ATOM 1526 CZ TYR 217 12	370 00 505
ANISOU 1526 CZ TYR 217 12	047 1.000 64.11
ATUM 152/ OF TVP 217 12	-1400 -017 - 2100
ANISOU 152/ OH TYR 217 11	040 5000 50.000 60.00
ATOM 1528 N ARG 218 14	.418 27.374 61 188 1 000 24 02
ANISOU 1528 N ARG 218 44	82 1611 3055 507 1477
ATOM 1529 CA ARG 218 15 ANISOU 1529 CA ARG 218 59	.335 28 465 60 949 1 000 70 71 71 45
3,000	32 2490 3245 -504 -1565 3.9.2
11770011 1 7 7 0 1 0	.326 28.135 59.840 1.000 35.00
3,000	59 2797 4562 -1397 -779 - 3 4 8
ATOM 1531 CG ARG 218 17 ANISOU 1531 CG ARG 218 600	27.114 60.073 1.000 35 77
ATOM 1532 CD ARG 218 18	$\frac{3087}{652} = \frac{4497}{377} = -1107 = 733 = 773$
ANISOU 1532 CD ARG 218 569	27.7/3 60.626 1.000 34.46
ATOM 1533 NE ARG 218 10	722 7242 -244 -619
ANISOU 1533 NE ARG 218 470	12 1-1000 29.51
ATOM 1534 CZ ARG 218 20.	218 28 620 59 830 1 830 33
ANISOU 1534 CZ ARG 218 526	3166 4170 60 450 1085
218 2U.	839 27.452 58.709 1 000 27 44
	2 2881 3341 -503 -373 -1505
	583 29.675 58.077 1.000 22.96
	$\frac{7}{1}$ $\frac{35}{9}$ $\frac{2817}{2817}$ $\frac{233}{233}$ $\frac{-1117}{117}$ $\frac{-872}{287}$
ANISOU 1537 C ARG 218 14. ANISOU 1537 C ARG 218 735	29.655 60.464 1.000 31.05
ATOM 1538 0 ARG 218 14	114 -1823 197
ANISOU 1538 O ARG 218 987	2011
ATUM 1539 N PRO 219 14	3433 331 -3168 - 627
AN1500 1539 N PRO 219 629	0 2559 2555 400 1030 004
ATOM 1540 CD PRO 219 14. ANISOU 1540 CD PRO 219 814	597 31.043 62 543 1 000 36 70
3 00 01 0 0 1 2	7 2878 2954 -1848 -2548 - 374
737700	464 31.841 60.549 1.000 26 34
ANISOU 1541 CA PRO 219 442 ATOM 1542 CB PRO 219 13.	2564 3025 -573 -988 - 340
ANISOU 1542 CB PRO 219 536	32.3 32.993 61.563 1.000 32.44
ATOM 1543 CG PRO 219 13	0.45 =0.13 -0.51 -41.1 - 9.8.9
ANISOU 1543 CG PRO 219 791	2 1 1 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
ATOM 1544 C PRO 219 14.	005 32.329 59 220 1 000 22 64
ANISOU 1544 C PRO 219 347	2 2066 3443 -161 1020 1 0 0
ANTIGOT 1515 0 FRO 219 13.	300 32.950 58.412 1 000 30 61
3 mov 4 = 1 = 1 = 1 = 1 = 1 = 1	$\frac{8}{2934}$ $\frac{2934}{4339}$ $\frac{4339}{-347}$ $\frac{-1712}{1712}$ $\frac{876}{171}$
ANISOU 1546 N ASP 330 361	²⁶⁹ 32.087 58.906 1.000 25.98
ATOM 1547 CA ASP 220 15	1 1/56 4506 -389 -644 - 815
ANISOU 1547 CA ASP 220 395	32.660 57.705 1.000 27.96
ATOM 1548 CB ASP 220 17	30 - 824
AN1300 1548 CB ASP 220 354	2110
ATUM 1549 CG ASP 220 18.0	091 32.158 58 780 1 000 72 00
ANISOU 1549 CG ASP 220 370 ATOM 1550 OD1 ASP 230 170	3527 4961 625 070 615
NTCOM 1550 351 MS1 220 17.8	597 31.434 59.719 1.000 26 12
	3522 3390 -158 -289 - 97
ANISOU 1551 OD2 ASP 220 19.2 ANISOU 1551 OD2 ASP 220 3714	32.088 58.281 1.000 29.09
ATOM 1552 C ASP 220 16 (3756 3581 304 677 - 712
ANISOU 1552 C ASP 220 2500	1201
ATOM 1553 O ASP 220 16.6	541 32.095 55 515 1 000 28 22
ANISOU 1553 O ASP 220 4088	1665 4994 955 200 424
ANT COT 155	500 30.510 56.631 1 000 21 58
7 mon	1770 3681 -288 178 -651
ANTCOM 1555 51 ADA 221 15.8	40 29.484 55.658 1.000 19.81
ATOM 1556 CB ALA 221 2986 ATOM 1556 CB ALA 221 17.1	$\frac{1452}{3090} -342 -224 -315$
221 1/.]	30 28.800 56.109 1.000 19.51

- 141 -ANISOU 1556 CB ALA 221 2267 1497 3647 -648 45 - 746 1557 C ALA 221 14.718 28.469 55.489 1.000 17.71 ATOM ANISOU 1557 C ALA 221 2304 1912 2512 -251 -75 -309 ATOM 1558 O ALA 221 13.866 28.356 56.380 1.000 20.97 ANISOU 1558 O ALA 221 3596 2029 2344 -503 406 -284 ATOM 1559 N VAL 222 14.728 27.756 54.378 1.000 14.22 ANISOU 1559 N VAL 222 1560 1582 2262 -76 -92 -11 ATOM 1560 CA VAL 222 13.823 26.617 54.160 1.000 14.89 ANISOU 1560 CA VAL 222 1326 1608 2723 98 -216 -205 ATOM 1561 CB VAL 222 13.079 26.779 52.830 1.000 17.28 ANISOU 1561 CB VAL 222 13.079 26.779 52.830 1.000 17.28 ANISOU 1562 CG1 VAL 222 13.995 26.685 51.620 1.000 19.17 ANISOU 1562 CG1 VAL 222 13.995 26.685 51.620 1.000 19.17 ANISOU 1563 CG2 VAL 222 1974 2625 2686 -446 -775 150 ANISOU 1563 CG2 VAL 222 11.996 25.747 52.641 1.000 17.36 ANISOU 1563 CG2 VAL 222 11.996 25.747 52.641 1.000 17.36 ANISOU 1564 C VAL 222 11.996 25.339 54.263 1.000 12.66 ANISOU 1565 O VAL 222 1136 1564 2112 -50 -225 -378 ANISOU 1565 O VAL 222 1136 1564 2112 -50 -225 -378 ANISOU 1565 O VAL 222 1136 1564 2112 -50 -225 -378 ANISOU 1565 O VAL 222 1288 1879 25.339 1.000 12.66 ANISOU 1566 N LEU 223 14.049 24.267 54.775 1.000 12.98 ANISOU 1566 N LEU 223 14.049 24.267 54.775 1.000 12.98 ANISOU 1567 CA LEU 223 14.681 22.952 54.749 1.000 10.70 ANISOU 1567 CA LEU 223 14.276 22.130 55.961 1.000 13.02 ANISOU 1557 C ALA 221 2304 1912 2512 -251 -75 -309 -13 -199 LEU 223 14.276 22.130 55.961 1.000 13.02 LEU 223 1387 1968 1593 -419 289 -ATOM 1568 CB ANISOU 1568 CB LEU 223 1387 -419 289 -108 LEU 223 14.739 20.683 56.106 1.000 17.41 LEU 223 2434 2132 2050 200 4765 1569 CG ANISOU 1569 CG LEU 223 2434 2132 2050 -290 -476 5 6 6 1570 CD1 LEU 223 16.247 20.614 56.204 1.000 17.20 1570 CD1 LEU 223 2576 1518 2441 26-989 -24 ATOM ANISOU 1570 CD1 LEU 223 2576 ATOM 1571 CD2 LEU 223 13.983 20.076 57.282 1.000 33.63 ANISOU 1571 CD2 LEU 223 3981 4721 4077 -341 134 2949 ATOM 1572 C LEU 223 14.362 22.211 53.456 1.000 10.02 ANISOU 1572 C LEU 223 1000 1265 1543 58 - 319 8 8 ATOM 1573 O LEU 223 13.206 22.160 53.088 1.000 12.86

ANISOU 1573 O LEU 223 949 1945 1992 -97 -174 -372

ATOM 1574 N VAL 224 15.406 21.675 52.798 1.000 10.55

ANISOU 1574 N VAL 224 978 1070 1962 -76 -418 -382

ATOM 1575 CA VAL 224 15.227 20.932 51.553 1.000 11.98

ANISOU 1575 CA VAL 224 1376 1288 1887 -249 -278 -372

ATOM 1576 CB VAL 224 16.095 21.461 50.391 1.000 11.23

ANISOU 1576 CB VAL 224 16.095 21.461 50.391 1.000 11.23

ANISOU 1576 CB VAL 224 15.833 20.690 49.102 1.000 13.16

ANISOU 1577 CG1 VAL 224 1899 1485 1615 -462 -5168 4

ATOM 1578 CG2 VAL 224 15.837 22.941 50.156 1.000 13.86

ANISOU 1578 CG2 VAL 224 15.837 22.941 50.156 1.000 13.86

ANISOU 1579 C VAL 224 15.539 19.450 51.786 1.000 10.87

ANISOU 1579 C VAL 224 15.539 19.450 51.786 1.000 10.87

ANISOU 1579 C VAL 224 15.539 19.450 51.786 1.000 10.87

ANISOU 1580 O VAL 224 1283 1363 2132 -175 -154 - 274

ATOM 1581 N PHE 225 14.585 18.553 51.533 1.000 11.86

ANISOU 1581 N PHE 225 1241 1128 2137 -15 -303 - 61

ATOM 1582 CA PHE 225 14.811 17.130 51.412 1.000 11.38 ATOM 1573 O LEU 223 13.206 22.160 53.088 1.000 12.86 225 1241 1128 2137 -15 -303 - 6 1 225 14.811 17.130 51.412 1.000 11.38 1582 CA MOTA PHE 225 1260 1157 1909 -22 -67 - 5 6 225 13.707 16.280 52.044 1.000 11.34 225 1117 1176 2015 205 -213 3 3 5 225 13.654 16.172 53.544 1.000 11.38 ANISOU 1582 CA PHE ATOM 1583 CB PHE ANISOU 1583 CB PHE 1584 CG MOTA PHE ANISOU 1584 CG PHE 225 964 1369 1991 225 964 1369 1991 -251 -333 181 225 14.685 15.653 54.291 1.000 15.28 1585 CD1 PHE ATOM 225 1771 1777 2256 -98 -853 2 225 12.532 16.576 54.254 1.000 17.91 225 1904 2748 2153 241 ANISOU 1585 CD1 PHE 2256 -98 -853 2 9 8 1586 CD2 PHE ANISOU 1586 CD2 PHE 225 1904

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- .142 -
                             1587 CE1 PHE 225 14.619 15.535 55.661 1.000 17.46
     ANISOU 1587 CE1 PHE 225 2449 1862 2321 -249 -795 66 ATOM 1588 CE2 PHE 225 12.447 16.474 55.612 1.000 19.35 ATOM 1589 CZ PHE 225 2563 2678 2111 121 129 -1 ANISOU 1589 CZ PHE 225 2952 1641 2324 -501 -470 3
      ANISOU 1587 CE1 PHE 225 2449
                                                                                                                                                                                                        -249 -795 6 6 6
                                                                                                                                                                                                                               129 - 11
ANISOU 1589 CZ PHE 225 14.907 16.774 49.927 1.000 12.03 PHE 325 14.019 17.160 49.163 1.000 12.77 ANISOU 1591 O PHE 325 14.019 17.160 49.163 1.000 12.77 ANISOU 1592 N CYS 226 15.940 16.032 49.521 1.000 9.6 2 ANISOU 1593 CA CYS 226 954 1403 1296 -204 -407 2 9 ANISOU 1593 CA CYS 226 15.917 15.400 48.197 1.000 10.80 ANISOU 1593 CA CYS 226 15.917 15.400 48.197 1.000 10.80 ANISOU 1594 CB CYS 226 15.39 1362 1666 -357 16 -12 5 ANISOU 1595 SG CYS 226 15.39 1362 1666 -357 16 -12 5 ANISOU 1595 SG CYS 226 1627 1400 2192 -341 18 13 9 ANISOU 1595 SG CYS 226 16.429 47.744 1.000 12.02 ANISOU 1595 CC CYS 226 14.98 14.178 48.256 1.000 9.86 ANISOU 1596 C CYS 226 1190 1061 1495 -20 -293 -1 6 ANISOU 1596 C CYS 226 15.015 13.431 49.252 1.000 11.17 ANISOU 1598 N GLY 227 14.217 13.963 47.205 1.000 11.17 ANISOU 1598 N GLY 227 14.217 13.963 47.205 1.000 11.17 ANISOU 1599 CA GLY 227 14.28 1010 1427 -258 -271 - 3 5 ANISOU 1599 CA GLY 227 14.38 717 1445 16 -35 16 9 ANISOU 1590 CA GLY 227 14.38 717 1445 16 -35 16 9 ANISOU 1600 C GLY 227 14.38 717 1445 16 -35 16 9 ANISOU 1601 O GLY 227 14.38 717 1445 16 -35 16 9 ANISOU 1602 N ALA 228 13.650 9.529 45.103 1.000 9.48 ANISOU 1600 C ALA 228 13.650 9.529 45.103 1.000 9.48 ANISOU 1603 CA ALA 228 13.650 9.529 45.103 1.000 9.40 ANISOU 1605 C ALA 228 13.55 87 19.91 446 150 9.01 4.77 1.000 9.48 ANISOU 1606 C ALA 228 13.55 887 1371 9 -74 - 35 10.000 9.48 ANISOU 1606 C ALA 228 13.650 9.529 45.103 1.000 9.48 ANISOU 1606 C ALA 228 13.650 9.529 45.103 1.000 9.48 ANISOU 1606 C ALA 228 13.650 9.529 45.103 1.000 9.48 ANISOU 1606 C ALA 228 13.650 9.529 45.103 1.000 9.48 ANISOU 1606 C ALA 228 13.650 9.529 45.103 1.000 9.48 ANISOU 1606 C ALA 228 13.650 9.529 45.103 1.000 9.48 ANISOU 1608 CA ALA 228 13.77 9.9147 1.000 9.25 ANISOU 1608 CA ALA 228 13.79 9.9147 1.000 9.25 ANI
     ANISOU 1589 CZ PHE 225 2952 1641 2324 -501 -470 3
ATOM 1590 C PHE 225 14.907 16.774 49.927 1.000 12.03
                                                                                                                                                                                                      -501 -470 3 6
                                                                                                                                      1446 1487 -2 -159 251
   ATOM 1609 CB ILE 229 11.802 12.078 41.295 1.000 11.52
ANISOU 1609 CB ILE 229 1257 1473 1647 34 -57 3 6 2
  ATOM 1610 CG2 ILE 229 1257 1473 1647 34 -57 3 6 2
ANISOU 1610 CG2 ILE 229 11.997 12.852 39.999 1.000 11.30
ATOM 1611 CG1 ILE 229 1655 1211 1426
                               1610 CG2 ILE 229 1655 1211 1426 83 -189 156
1611 CG1 ILE 229 10.575 11.131 41.237 1.000 14.39
  ANISOU 1611 CG1 ILE 229 1031
                               1611 CG1 ILE 229 1031 2034 2402 -40 210 3
1612 CD1 ILE 229 10.676 10.093 40.138 1.000 19.20
                                                                                                                                                                                                  -40 210 311
   ATOM
  ANISOU 1612 CD1 ILE 229 2085 1723
                                                                                                                                                                     3489 -610 93 -138
                              1613 C ILE 229 14.389 12.034 41.477 1.000 10.38
   ATOM
   ANISOU 1613 C
                                                                ILE 229 1293
 ATOM 1613 C ILE 229 1293 1405 1247 -62 -169 3 2 2 ATOM 1614 O ILE 229 14.952 11.947 40.369 1.000 11.66 ATOM 1615 N ALA 230 14.965 12.692 42.490 1.000 10.66 ATOM 1616 CA ALA 230 1476 1274 1300 -104 -151 3 5 6 ANISOU 1616 CA ALA 230 16.312 13.259 42.338 1.000 11.21 ATOM 1617 CB ALA 230 16.681 14.148 43.509 1.000 10.58
                                                                                                                                      1405
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- 143 -
 ANISOU 1617 CB ALA 230 1350 1295 1375 62-106 12 ATOM 1618 C ALA 230 17.336 12.136 42.132 1.000 11.28 ANISOU 1618 C ALA 230 1640 1037 1610 1 55 2 4 2 ATOM 1619 O ALA 230 18.220 12.185 41.273 1.000 11.29
                                                        1375 62 - 106 1 2 6
 ANISOU 1619 O
                       ALA
                             230 1510 1240 1539 -189 -40 288
231 17.173 11.097 42.946 1.000 10.55
          1620 N
 MOTA
                       THR
 ANISOU 1620 N
                              231 1328 894 1787 -262 -70 2 1 4
231 18.064 9.939 42.819 1.000 11.98
                       THR
          1621 CA
                      THR
 ATOM
 ANISOU 1621 CA
                       THR
                              231 1929 1018 1605 0 -164 15 231 17.717 8.865 43.878 1.000 10.76
                                                        1605 0 -164 159
          1622 CB
                       THR
 ATOM
 ANISOU 1622 CB
                             231 1381 1070 1636 -86 -453 2
231 17.658 9.437 45.198 1.000 11.82
                       THR
                                                                    -86 -453 2 4 6
          1623 OG1 THR
 ATOM
          1623 OG1 THR 231 17.658 9.437 45.198 1.000 11.82 1623 OG1 THR 231 1615 1236 1641 35 -115 2 7 7 1624 CG2 THR 231 18.765 7.752 43.880 1.000 12.57 1624 CG2 THR 231 1621 1314 1840 160 -89 3 1625 C THR 231 17.958 9.352 41.415 1.000 12.52 1625 C THR 231 1632 1500 1624 -145 42 1 1
 ANISOU 1623 OG1 THR
                                                                    35 -115 277
 MOTA
 ANISOU 1624 CG2 THR
                                                                    160 -89 351
 MOTA
 ANISOU 1625 C
          1625 C THR 231 1632 1500 1624 -145 42 1 1 1626 O THR 231 18.939 9.050 40.732 1.000 12.15
 ATOM
 ANISOU 1626 O
                   THR 231 1636
                                               1233
ANISOU 1626 O THR 231 1636 1233 1747 -17 86 2 2 4 ATOM 1627 N LEU 232 16.717 9.154 40.959 1.000 11.14 ANISOU 1627 N LEU 232 1608 1005 1620 90 -68 1 4 1 ATOM 1628 CA LEU 232 16.446 8.522 39.675 1.000 12.47 ANISOU 1628 CA LEU 232 1880 1203 1657 109 -169 4 ATOM 1629 CB LEU 232 14.950 8.214 39.552 1.000 12.81 ANISOU 1629 CB LEU 232 1989 1225 1654 -78 -209 1
                                                         1747
                                                                    -17 86 2 2 4
                                                                          -169 4 5
                                                                          -209 1 9
ATOM 1630 CG LEU 232 14.452 7.464 38.314 1.000 14.85
ANISOU 1630 CG LEU 232 2171 1753 1719 -5 -410 -9 (
ATOM 1631 CD1 LEU 232 15.020 6.055 38.240 1.000 16.78
                                                                    -5 -410 - 96
 ANISOU 1631 CD1 LEU 232-2693 1749 1932 72-431 -487
          1632 CD2 LEU 232 12.914 7.411 38.291 1.000 15.70
ANISOU 1632 CD2 LEU 232 2180 1866 1920
 ANISOU 1642 N
                      THR 234 1457 1639 1893 -139 223 1 2 6
                             234 20.613 11.930 38.244 1.000 13.00
          1643 CA THR
 MOTA
 ANISOU 1643 CA THR
                             234 1483 1600
                                                          1855 -188 428 1 4 3
                             234 21.069 12.726 39.465 1.000 12.46
 ATOM
          1644 CB THR
 ANISOU 1644 CB
                      THR
                             234 1300 1632 1803 -32 200 251
          1645 OG1 THR
 MOTA
                             234 20.825 11.941 40.639 1.000 13.71
 ANISOU 1645 OG1 THR
                             234 1660 1662 1888 192 202 291
                             234 20.301 14.027 39.643 1.000 11.37
          1646 CG2 THR
 ANISOU 1646 CG2 THR
                             234 1097 1565 1657 -153 -87 169
          1647 C
                             234 21.424 10.643 38.178 1.000 14.44
                       THR
 ANISOU 1647 C
                       THR
                             234 1550 1823 2114
                                                                 6 -73 - 53
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ATOM 1648 O	THR 2	34 22.659	10.710	38.233	1.000 15.81
ANISOU 1648 O ATOM 1649 N	THR 2	34 1546	2169	2293	61 27 2 1 7
ATOM 1649 N ANISOU 1649 N	GLY 2 GLY 2	35 20.767		38.070	1.000 14.76
ATOM 1650 CA		35 1776	1576	2254	77 81 410
ANISOU 1650 CA		35 21.530 35 2053		37.994	1.000 16.69
ATOM 1651 C		35 2053 35 22.243	1803 7.862	2486	304 35 189
ANISOU 1651 C	_	35 1854	2031	39.275 2512	1.000 16.83
ATOM 1652 O	GLY 2	35 23.305	7.237	39.194	765 244 193
ANISOU 1652 O	GLY 2	35 2074	2172	3225	1.000 19.67 1035 383 372
ATOM 1653 N ANISOU 1653 N	GLY 2	36 21.665	8.227	40.425	1035 383 372 1.000 14.46
ATOM 1654 CA	GLY 2 GLY 2	36 1732	1327	2433	154 198 7 5
ANISOU 1654 CA		36 22.187 36 2060		41.692	1.000 15.73
ATOM 1655 C		36 23.166	1381 8.691	2536	41 186 3 1 2
ANISOU 1655 C		36 1931	1332	42.388 2346	1.000 14.76
ATOM 1656 O	GLY 2	36 23.778	8.244	43.373	252 73 2 8 8 1.000 18.32
ANISOU 1656 O ATOM 1657 N	GLY 2	36 1983	2197	2782	106 -105 8 4 4
ANISOU 1657 N	GLN 2	37 23.318	9.938	41.953	1.000 13.99
ATOM 1658 CA		37 1831	1349	2137	158 165 170
ANISOU 1658 CA		37 24.209 37 1474	10.956	42.485	1.000 13.13
ATOM 1659 CB		37 24.629	1304 11.948	2210	367 -31 276
ANISOU 1659 CB	GLN 2:	37 1367	1566	41.383 2151	1.000 13.38
ATOM 1660 CG ANISOU 1660 CG	GLN 23	7 25.390	11.335	40.219	99 72 159 1.000 14.74
ATOM 1661 CD	GLN 23	7 1404	1529	2666	518 410 333
ANISOU 1661 CD	GLN 23 GLN 23	7 25.816	12.428	39.257	1.000 17.22
ATOM 1662 OF 1	GIM 23	7 2039 7 26.754	2018	2486	-64 426 360
ANISOU 1662 OE1	GLN 23	7 1566	13.208 2334	39.522	1.000 20.60
ATOM 1663 NE2	GLN 23	7 25.116	12.470		-10 -29 965
ANISOU 1663 NE2	CLN 23	7 2014	2093		1.000 17.47 208 438 408
ATOM 1664 C ANISOU 1664 C	GLN 23	7 23.627	11.739		208 438 408 1.000 12.90
ATOM 1665 O		7 1474	1324		72 -10 2 5 5
ANISOU 1665 O		7 24.332 7 1739	12.549	44.282	1.000 15.90
ATOM 1666 N		8 22.365	1888 11.481		-291 74 - 84
ANISOU 1666 N	VAL 23	8 1372	962 227	44.013 76 212	1.000 12.13
ATOM 1667 CA	VAL 23	8 21.664	12.182		-33 2 0 0 1.000 11.91
ANISOU 1667 CA ATOM 1668 CB	VAL 23	8 1169	1436		-121 -276 - 19
ANISOU 1668 CB	VAL 23 VAL 23	8 20.622	13.158	44.510	1.000 12.00
ATOM 1669 CG1	VAL. 23	8 1024 8 19.978	1179	2357	-6 199 - 3 1
ANISOU 1669 CG1	VAL 23	8 1530		45.601	1.000 13.07
ATOM 1670 CG2	7721 22	8 21.207	14.088	1767	63 -232 -222
ANISOU 1670 CG2 ATOM 1671 C	VAL 23	8 1795	1470		1.000 14.00 -40 -2 181
ATOM 1671 C ANISOU 1671 C	VAL 23	8 20.990	11.156		1.000 13.62
ATOM 1672 O	VAL 23 VAL 23	8 1707	1415	2054 -	-103 -40 -22
ANISOU 1672 O	VAL 23	8 20.252 8 1702	10.288	45.492	1.000 12.64
ATOM 1673 N		9 21.247	977 212 11.246		-318 257
ANISOU 1673 N	LYS 23	9 1075		47.300 : 2076 : :	1.000 11.99
ATOM 1674 CA	LYS 23	9 20.568			127 -101 7 4 1.000 12.77
ANISOU 1674 CA ATOM 1675 CB	LYS 23	9 1224	1541		-12 -124 8 6
ATOM 1675 CB ANISOU 1675 CB	LYS 23 LYS 23	9 21.382	10.463		1.000 12.23
ATOM 1676 CG		9 1333	1155	2158	L83 -234 - 28
ANISOU 1676 CG		9 20.953 9 1643			L.000 13.85
ATOM 1677 CD		9 21.927			L87 -52 -89
ANISOU 1677 CD	LYS 23	9 2893		51.957 <u>1</u> 2961 <u>1</u>	L.000 20.13
ATOM 1678 CE	LYS 23	9 21.364			LO -1185 5 8 8 L.000 24.73

					- 145 -		-
ANISOU			LYS	239 4065	2250	3080	-348 -1466 1064
ATOM	1679		LYS	239 22.019	8.841		1.000 32.28
ANISOU			LYS	239 5658	4315	2293	1610 -930 - 304
ATOM	1680		LYS	239 19.169	10.949	48.661	
ANISOU			LYS	239 1207	1332	1866	-35 -82 6 4
ATOM	1681		LYS	239 18.976	12.191	48.708	
ANISOU			LYS	239 1638	1294	1749	-2 -25 2 3 6
ATOM	1682		ALA	240 18.222	10.047	48.863	
ANISOU			ALA	240 1248	1266	1534	-52 -185 - 88
ATOM	1683		ALA	240 16.884	10.368	49.354	
ANISOU			ALA	240 1292	1057	1531	-195 -37 -109
ATOM	1684		ALA	240 15.784	9.782	48.466	1.000 13.46
ANISOU			ALA	240 1195	2378	1543	-232 20 - 403
ATOM	1685		ALA	240 16.784	9.881	50.807	1.000 10.97
ANISOU			ALA	240 1308	1249	1611	-127 -142 4 9
ATOM	1686	0	ALA	240 16.595	8.664	51.059	1.000 13.02
ANISOU			ALA	240 2136	1242	1568	-243 . 28 - 7
ATOM	1687		PRO	241 16.967	10.783	51.782	1.000 11.13
ANISOU			PRO	241 1723	1041	1466	160 -49 138
ATOM	1688		PRO	241 17.172	12.237	51.654	1.000 11.17
ANISOU			PRO	241 1419	1204	1618	-180 -128 7 6
ATOM	1689		PRO	241 17.043	10.340	53.166	1.000 11.96
ANISOU			PRO	241 1597	1447	1499	-172 - 32 193
ATOM	1690	CB	PRO	241 17.712	11.545	53.891	1.000 14.25
ANISOU			PRO	241 1875	1837	1701	-531 -383 2 4 2
ATOM	1691	CG	PRO	241 17.286	12.724	53.069	1.000 13.61
ANISOU ATOM	1691		PRO	241 2015	1446	1709	-596 -465 - 22
ANISOU	1607		PRO	241 15.708	10.072	53.861	1.000 12.35
ATOM	1693		PRO	241 1417	1610	1665	-175 -187 4 1 8
ANISOU	1603	0	PRO	241 14.759	10.829	53.655	1.000 12.28
ATOM	1694		PRO	241 1359	1582	1723	-232 -468 8 1
ANISOU	1694	M	ARG ARG	242 15.700 242 1775	9.033	54.711	1.000 12.75
ATOM	1695		ARG	242 17/5	1407	1664	-170 76 2 5 0
ANISOU	1695	CA	ARG	242 14.563	8.804	55.576	1.000 10.76
ATOM	_	CB	ARG	242 1292	1417	1380	-207 -281 2 1 1
ANISOU		CB	ARG	242 2419	7.405	56.223	1.000 15.02
ATOM	1697		ARG	242 2419	1368 6.342	1918	-357 117 294
ANISOU			ARG	242 3373	1274	55.230 2135	1.000 17.85
ATOM	1698	CD	ARG	242 14.254	4.934		9 -560 251 1.00019.42
ANISOU			ARG	242 3148	1111	3120	506 503 116
ATOM	1699	NE	ARG	242 15.667		55.849	1.000 20.71
ANISOU			ARG	242 3225	2107	2538	938 638 212
\mathtt{ATOM}	1700	CZ	ARG	242 16.107	3.444	56.416	1.000 23.22
ANISOU			ARG	242 3198	2206	3417	307 -544 5 8 9
ATOM	1701	NH1	ARG	242 15.285	2.567	56.980	1.000 24.46
ANISOU	1701	NH1	ARG	242 4097	2112	3083	307 387 195
ATOM	1702	NH2	ARG	242 17.416	3.184		1.000 25.41
ANISOU	1702	NH2		242 3402	2332	3921	819 -267 4 0 3
ATOM	1703	С	ARG	242 14.477	9.834	56.704	1.000 11.95
ANISOU			ARG	242 1571	1463	1506	-248 -214 1 0 7
ATOM	1704	0	ARG	242 15.469	10.377	57.213	1.000 13.65
ANISOU			ARG	242 1708	1439	2040	-322 -401 - 38
ATOM	1705		HIS	243 13.252	10.085	57.118	1.000 11.60
ANISOU ATOM			HIS	243 1657	1410	1342	-311 -206 5
ANISOU	1706	CA	HIS	243 12.942	11.056		1.000 11.49
ANISOU			HIS	243 1855	1571	938 -30	
ANISOU	1707		HIS	243 12.968	12.462	57.546	1.000 11.22
ATOM	1707		HIS	243 1432	1379	1453	-231 -221 3 9
ANISOU	1700	CC	HIS	243 12.133	12.694	56.341	1.000 11.80
	1,00	CG	HIS	243 1937	1171	1378	-31 -268 7 9

- 146 -1709 CD2 HIS 243 10.885 13.236 56.181 1.000 11.15 ATOM ANISOU 1709 CD2 HIS 243 1990 1106 1142 35 - 344 141 1710 ND1 HIS 243 12.538 12.345 55.086 1.000 12.29 ANISOU 1710 ND1 HIS 243 1670 1606 1395 -394 -91 8 MOTA 1711 CE1 HIS 243 11.599 12.653 54.209 1.000 12.59 ANISOU 1711 CE1 HIS 243 1686 1740 1357 -522 -202 -2531712 NE2 HIS MOTA 243 10.585 13.204 54.841 1.000 10.77 ANISOU 1712 NE2 HIS 243 1612 1307 1172 -616 -268 - 36 1713 C ATOM HIS 243 11.605 10.737 58.812 1.000 12.49 ANISOU 1713 C HIS 243 1869 1570 1308 -321 -53 7 3 1714 0 ATOM HIS 243 10.807 9.949 58.271 1.000 12.26 ANISOU 1714 O HIS 243 1756 1404 1497 -188 -115 4 7 ATOM 1715 N HIS 244 11.352 11.319 59.983 1.000 12.16 ANISOU 1715 N HIS 244 1464 1715 1442 244 1464 1/15 1442 -250 -112 244 10.138 11.043 60.758 1.000 12.02 -230 -112 - 3 2 1716 CA ATOM HIS ANISOU 1716 CA 244 1606 HIS 1809 1152 -599 -167 - 241717 CB 244 10.255 HIS 9.778 61.615 1.000 12.51 ANISOU 1717 CB HIS 244 1655 1763 1334 -19 101 - 47 1718 CG HIS 244 11.270 9.810 62.698 1.000 15.04 ANISOU 1718 CG 244 2025 HIS 1723 1965 -178 -433 1 5 4 1719 CD2 HIS ATOM 244 11.276 10.380 63.923 1.000 18.19 ANISOU 1719 CD2 HIS 244 2946 2339 1627 36 - 732 297 1720 ND1 HIS 244 12.504 9.203 62.662 1.000 19.30 ANISOU 1720 ND1 HIS 244 2303 2232 2800 229 -708 2 6 6 ATOM 1721 CE1 HIS 244 13.226 9.387 63.731 1.000 22.48 ANISOU 1721 CE1 HIS 244 2649 11 -1206 6 5 0 2734 3159 1722 NE2 HIS 244 12.476 10.120 64.531 1.000 22.33 ANISOU 1722 NE2 HIS 244 3088 2895 2500 -272 -1236 384 MOTA 1723 C HIS 244 9.780 12.246 61.613 1.000 13.47 ANISOU 1723 C HIS 244 1897 1673 1549 -362 254 6 7 1724 0 MOTA HIS 244 10.603 13.165 61.798 1.000 13.48 ANISOU 1724 O HIS 244 1800 1726 1595 -283 139 -161 ATOM 1725 N VAL 245 8.551 12.245 62.130 1.000 15.26
VAL 245 1852 1964 1983 -417 232 -55
VAL 245 8.090 13.352 62.970 1.000 17.31
VAL 245 2108 2442 2026 -125 476 -161
VAL 245 6.939 14.169 62.360 1.000 17.33
VAL 245 2094 2473 2019 -80 340 -477
VAL 245 6.551 15.334 63.286 1.000 25.25
VAL 245 2217 2966 4410 -137 1939 -1248
VAL 245 7.252 14.713 60.966 1.000 21.49
VAL 245 7.252 14.713 60.966 1.000 21.49
VAL 245 7.682 12.768 64.327 1.000 18.29
VAL 245 7.682 12.768 64.327 1.000 18.29
VAL 245 6.765 11.945 64.429 1.000 18.62
VAL 245 1810 2174 3089 -15 451 254
ALA 246 8.385 13.202 65.369 1.000 21.54
ALA 246 8.385 3045 2327 -591 -407 9 0 7
ALA 246 8.133 12.701 66.719 1.000 25.10 VAL 245 8.551 12.245 62.130 1.000 15.26 ANISOU 1725 N ATOM 1726 CA .VAL ANISOU 1726 CA 1727 CB ANISOU 1727 CB 1728 CG1 VAL ANISOU 1728 CG1 VAL -137 1939 - 1248 MOTA 1729 CG2 VAL ANISOU 1729 CG2 VAL ATOM 1730 C ANISOU 1730 C 1731 0 ATOM ANISOU 1731 O ATOM 1732 N ANISOU 1732 N 1733 CA ALA 246 8.133 12.701 66.719 1.000 25.10 1733 CA ALA 246 4596 2562 2379 94 -225 9.97 ATOM ANISOU 1733 CA 94 - 225 9 9 7 ATOM 1734 CB ALA 246 9.424 12.723 67.537 1.000 29.82 ANISOU 1734 CB ALA 246 5381 3408 2540 402 -889 1 3 2 5 ATOM 1735 C ALA 246 7.080 13.545 67.412 1.000 31.20 ANISOU 1735 C ALA 246 5079 4143 2632 314 280 428 MOTA 1736 0 ALA 246 6.876 14.714 67.052 1.000 32.39 ANISOU 1736 O ALA 246 4706 3748 3853 567 1247 - 66 MOTA 1737 N ALA 247 6.429 12.973 68.413 1.000 37.30 ANISOU 1737 N ALA 247 5548 5498 3126 92 640 8 3 5 ATOM 1738 CA ALA 247 5.585 13.794 69.271 1.000 40.42 ANISOU 1738 CA ALA 247 5434 6048 3878 15 1313 8 5 0 ATOM 1739 C ALA 247 6.289 14.132 70.578 1.000 42.17

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ANISOU 1739 C
               ALA 247 6495
                                5891
                                       3636
                                              -823 1720 3 4 1
       1740 O
               ALA 247 7.048
                                13.338 71.136 1.000 41.63
ANISOU 1740 O
                   247 5811
               ALA
                               6371
                                       3637
                                              -1631 804 425
       1741 CB
               ALA
                    247 4.280
                                13.067 69.525 1.000 47.17
ANISOU 1741 CB' ALA
                    247 5186
                               9059
                                       3676
                                              -520 523 2683
ATOM
       1742 N
                    257 1.781
               SER
                                21.848 70.382 1.000 31.02
ANISOU 1742 N
                    257 4109
               SER
                               5558
                                       2119
                                              137 -235 -810
       1743 CA
MOTA
                    257 1.214
               SER
                                21.932 69.052 1.000 27.01
ANISOU 1743 CA
               SER
                    257 2792
                                       2304
                                5165
                                              109 -143 - 707
       1744 CB
ATOM
                    257 0.039
               SER
                                22.914 68.992 1.000 28.16
ANISOU 1744 CB
               SER
                    257 2655
                               4473
                                       3572
                                              -238 -90 -1071
MOTA
       1745 OG
               SER
                    257 0.491
                                24.251 69.074 1.000 51.32
ANISOU 1745 OG
               SER
                    257 8516
                               4131
                                       6853
                                              -616 - 2734 - 807
       1746 C
ATOM
               SER
                    257 2.259
                                22.389 68.034 1.000 26.19
ANISOU 1746 C
               SER
                    257 2537
                                5064
                                       2 3 5.0
                                              -132 -413 -527
       1747 0
MOTA
               SER 257 3.286
                                22.938 68.352 1.000 31.47
ANISOU 1747 O
               SER 257 2740
                               5886
                                       3330
                                              -435 -689 -639
       1748 N
               ARG 258 2.022 22.123 66.763 1.000 26.04
ATOM
ANISOU 1748 N
               ARG 258 3257
                               4477
                                       2161
                                              -238 -441 - 19
ATOM
       1749 CA
               ARG
                    258 2.982
                               22.541 65.747 1.000 25.81
ANISOU 1749 CA
                    258 2606
               ARG
                               4735
                                      2466
                                              73 - 338 - 197
       1750 C
ATOM
               ARG
                    258 2.321
                               22.609 64.383 1.000 18.26
ANISOU 1750 C
               ARG
                    258 2374
                               2541
                                      2021
                                              39 83 - 854
       1751 0
ATOM
               ARG
                    258 1.288
                               21.967 64.131 1.000 19.23
ANISOU 1751 O
                    258 2600
               ARG
                               2819
                                       1883
                                              -389 311 -420
ATOM
      1752 CB
               ARG
                    258 4.188
                               21.592 65.664 1.000 29.78
ANISOU 1752 CB
               ARG
                    258 3403
                               5052
                                       2861
                                              695
                                                    -552 - 57
      1753 CG
ATOM
               ARG
                    258 4.246
                               20.784 64.384 1.000 32.64
ANISOU 1753 CG
               ARG
                    258 4358
                               4148
                                       3896
                                              146
                                                   97 - 561
      1754 CD
ATOM
               ARG
                    258 5.325
                               19.746 64.499 1.000 30.38
ANISOU 1754 CD
               ARG
                    258 3812
                                4423
                                       3309
                                              -57
                                                    341 - 16
ATOM
      1755 NE
               ARG
                    258 6.433
                               19.909 63.581 1.000 29.43
ANISOU 1755 NE
               ARG
                    258 3990
                                4604
                                       2588
                                              -22
                                                    70 5 4 2
      1756 CZ
ATOM
               ARG
                    258 6.453
                               19.389 62.359 1.000 25.02
ANISOU 1756 CZ
               ARG
                    258 2540
                               3893
                                       3074
                                              304
                                                    -243 1 0 4
ATOM
      1757 NH1 ARG
                    258 5.456
                               18.677 61.835 1.000 22.88
ANISOU 1757 NH1 ARG
                    258 2105
                               2607
                                       3982
                                              359
                                                    315 289
ATOM
      1758 NH2 ARG
                    258 7.523
                               19.593 61.617 1.000 22.03
ANISOU 1758 NH2 ARG
                    258 2477
                               2775
                                       3120
                                              -430
                                                   -287 - 964
ATOM
      1759 N
                    259 2.927
               THR
                               23.415 63.527 1.000 20.17
ANISOU 1759 N
               THR 259 2010
                               3640
                                       2013
                                              -743 91 -1001
      1760 CA THR 259 2.485
                               23.505 62.138 1.000 18.33
ANISOU 1760 CA
               THR 259 1801
                               3043
                                       2121
                                              -533 43 -685
ATOM
       1761 CB
               THR 259 1.821
                               24.821 61.713 1.000 23.23
ANISOU 1761 CB
                    259 2082
               THR
                               3169
                                       3576
                                              -384 -164 - 580
      1762 OG1 THR
ATOM
                    259 2.839
                               25.830 61.681 1.000 34.27
ANISOU 1762 OG1 THR
                    259 2181
                               2562
                                      8277
                                              -137 -996 - 794
       1763 CG2 THR
ATOM
                    259 0.738
                               25.198 62.704 1.000 25.49
ANISOU 1763 CG2 THR
                    259 4466
                               2233 2987
                                              325
                                                    396 - 948
ATOM
      1764 C
                    259 3.702
               THR
                               23.352 61.222 1.000 18.44
ANISOU 1764 C
               THR
                    259 2035
                                      2150
                               2822
                                              -753 274 -583
ATOM
       1765 O
               THR
                    259 4.835
                               23.698 61.603 1.000 24.74
ANISOU 1765 O
               THR
                    259 1961
                               5370 2069
                                              -964 231 -714
ATOM
       1766 N
               SER
                    260 3.420
                               22.867 60.026 1.000 16.29
ANISOU 1766 N
               SER
                    260 1971
                                       1864
                               2352
                                              -224 2 - 75
       1767 CA SER
                    260 4.447
                               22.832 58.989 1.000 17.43
ANISOU 1767 CA SER
                    260 1783
                                       1879
                               2961
                                              321
                                                    -95 - 72
ATOM
       1768 CB
              SER
                    260 5.224
                                21.514 58.956 1.000 20.17
ANISOU 1768 CB
                    260 2306
               SER
                                3257
                                       2100
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       1769 OG
               SER
                    260 4.416
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ANISOU 1769 OG
                   260 3651
               SER
                                2803
                                       3839
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                                                    217 554
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- 148 -
                                                                                                                                                                                                      -190 -120 - 500
                                                                                                                                                                                                     -204 30 - 315
                                                                                                                                                                                                    -42 -240 - 161
                                                                                                                                                                                                    -68 -331 - 343
                                                                                                                                                                                                     -399 -485 - 318
                                                                                                                                                                                                     -719 -821 9 5 5
                                                                                                                                                                                                    156 -103 1 7
   ATOM 1780 CB VAL 262 5.026 19.639 53.558 1.000 11.87
ANISOU 1780 CB VAL 262 1262 1636 1614 9 -187 - 7
                                                                                                                                                                                                     9 -187 - 74
ATOM 1781 CG1 VAL 262 5.778 18.577 52.779 1.000 13.12

ANISOU 1781 CG1 VAL 262 1462 1527 1997 -2 185 5 1

ATOM 1782 CG2 VAL 262 5.262 19.564 55.062 1.000 17.08

ANISOU 1782 CG2 VAL 262 5.262 19.564 55.062 1.000 17.08

ANISOU 1783 C VAL 262 5.096 21.149 51.543 1.000 11.18

ATOM 1783 C VAL 262 1026 1790 1431 1 -111 -138

ATOM 1784 O VAL 262 3.939 20.969 51.127 1.000 12.76

ANISOU 1785 N PHE 263 6.090 21.438 50.714 1.000 9.50

ATOM 1785 N PHE 263 995 1297 1316 -6 -210 -181

ATOM 1786 CA PHE 263 5.933 21.637 49.288 1.000 9.61

ANISOU 1786 CA PHE 263 5.933 21.637 49.288 1.000 9.61

ANISOU 1787 CB PHE 263 6.486 23.002 48.848 1.000 9.61

ANISOU 1787 CB PHE 263 6.486 23.002 48.848 1.000 10.94

ANISOU 1787 CB PHE 263 6.150 23.399 47.418 1.000 10.94

ANISOU 1788 CG PHE 263 6.150 23.399 47.418 1.000 10.35

ANISOU 1788 CG PHE 263 6.858 22.915 46.326 1.000 9.98

ANISOU 1789 CD1 PHE 263 6.530 23.399 47.418 1.000 10.35

ANISOU 1789 CD2 PHE 263 6.530 23.399 47.418 1.000 10.35

ANISOU 1789 CD2 PHE 263 6.530 23.399 47.418 1.000 10.35

ANISOU 1789 CD2 PHE 263 6.530 23.399 47.418 1.000 10.94

ANISOU 1789 CD2 PHE 263 5.106 24.277 47.148 1.000 11.95

ANISOU 1790 CD2 PHE 263 5.106 24.277 47.148 1.000 11.95

ANISOU 1790 CD2 PHE 263 5.491 24.112 44.762 1.000 12.49

ANISOU 1791 CE1 PHE 263 6.530 23.229 45.019 1.000 12.49

ANISOU 1793 CZ PHE 263 1318 1453 1948 -138 -187 6 4 9

ANISOU 1793 CZ PHE 263 1318 1453 1948 -138 -187 6 4 9

ANISOU 1794 C PHE 263 1318 1453 1948 -138 -187 6 4 9

ANISOU 1795 O PHE 263 7.868 20.406 48.538 1.000 10.98

ATOM 1796 N PHE 264 5.856 19.691 47.812 1.000 9.19

ANISOU 1796 N PHE 263 6.386 20.505 48.530 1.000 9.92

ANISOU 1797 CA PHE 263 1868 20.406 48.538 1.000 10.98

ATOM 1797 CA PHE 263 1886 20.406 48.538 1.000 10.98

ATOM 1797 CA PHE 264 5.886 19.691 47.812 1.000 9.19

ANISOU 1797 CA PHE 264 5.886 19.691 47.812 1.000 9.19

ANISOU 1798 CB PHE 264 5.886 19.691 47.812 1.000 9.19

ANISOU 1799 CB PHE 264 5.886 19.691 47.812 1.000 9.92

ANISOU 1799 CB PHE 264 5.886 19.691 47.812 1.000 9.92

ANISOU 1799 CB PHE 264
   ATOM 1781 CG1 VAL 262 5.778 18.577 52.779 1.000 13.12
   ANISOU 1781 CG1 VAL 262 1462
                                                                                                                                  1527
                                                                                                                                                                                                     -2 185 5 1
                                                                                                                                                                     1648 -251 -84 -271
                                                                                                                                                                                                    -120 -224 - 145
                                                                                                                                  1238 1417 -56 -60 -126
  ANISOU 1798 CB PHE 264 1209 1201 1359 -78 17 9

ATOM 1799 CG PHE 264 5.265 16.673 48.336 1.000 11.22

ANISOU 1799 CG PHE 264 1241 1647 1374 -121 38 7 7
   ANISOU 1798 CB
                                                                                                                                   1647 1374 -121 38 7 7
   MOTA
                              1800 CD1 PHE
                                                                                    264 6.292
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- 149 -ANISOU 1800 CD1 PHE 264 1467 2641 1734 -225 -8 8 7 3 1801 CD2 PHE 264 3.988 16.433 48.808 1.000 16.96 ANISOU 1801 CD2 PHE 264 1425 3252 1769 -610 -79 958 1802 CE1 PHE 264 6.090 15.596 50.336 1.000 14.52 ANISOU 1802 CE1 PHE 264 1745 2417 1354 162 334 ATOM 1803 CE2 PHE 15.796 50.019 1.000 18.04 264 3.755 ANISOU 1803 CE2 PHE 264 1747 3405 1704 -590 -109 1008 1804 CZ PHE ATOM 264 4.817 ~15.354 50.779 1.000 12.52 ANISOU 1804 CZ PHE 1536 1449 -57 227 3 19.038 45.533 1.000 8.98 264 1772 1805 C PHE ATOM 264 6.535 ANISOU 1805 C PHE 264 1103 919 1392 143 81 - 92 PHE 264 5.497 19.368 44.930 1.000 9.79 1806 0 MOTA ANISOU 1806 O PHE 264 991 1190 1540 28 105 1 0 3 ATOM 1807 N ANISOU 1807 N LEU 265 7.758 19.031 44.999 1.000 8.43 ANISOU 1807 N LEU 265 992 884 1325 173 -180 158 ATOM 1808 CA LEU 265 7.984 19.224 43.566 1.000 8.66 ANISOU 1808 CA LEU 265 883 1066 1339 63 -33 - 76 ATOM 1809 CB LEU 265 9.309 19.964 43.328 1.000 10.10 ATOM 1809 CB LEU 265 9.309 19.964 43.328 1.000 10.10
ANISOU 1809 CB LEU 265 1179 1188 1469 -225 -220 24
ATOM 1810 CG LEU 265 9.570 20.351 41.871 1.000 9.37
ANISOU 1810 CG LEU 265 1072 1009 1478 242 25 1 29
ATOM 1811 CD1 LEU 265 8.725 21.522 41.408 1.000 10.80
ANISOU 1811 CD1 LEU 265 1291 1004 1811 181 -114 29
ATOM 1812 CD2 LEU 265 11.048 20.684 41.678 1.000 10.87
ANISOU 1812 CD2 LEU 265 1129 1483 1519 134 43 1 4 6
ATOM 1813 C LEU 265 7.933 17.849 42.875 1.000 10.21
ANISOU 1813 C LEU 265 932 1188 1760 -6 -38 -302 -225 -220 2 4 8 -114 2 9 6 ANISOU 1813 C LEU LEU 265 8.858 17.043 43.042 1.000 10.45 LEU 265 1388 969 1612 84 -217 107 ATOM 1814 0 ANISOU 1814 O LEU 265 1388 ARG 266 6.853 ATOM 1815 N 17.530 42.135 1.000 10.00 ANISOU 1815 N ARG 266 1325 1069 1404 -120 -222 1 5 16.198 41.628 1.000 10.50 1816 CA ARG 266 6.572 MOTA ANISOU 1816 CA ARG 266 1219 1816 CA ARG 266 1219 1217 1554 -294 110 -210 1817 CB ARG 266 5.208 15.675 42.124 1.000 10.56 ATOM ANISOU 1817 CB ARG 266 978 1460 1574 -168 -103 -105 1818 CG ARG 266 4.965 15.894 43.609 1.000 11.24 ANISOU 1818 CG ARG 266 1337 1373 1563 -40 119 206 1819 CD ARG 266 3.668 15.318 44.146 1.000 11.17 ATOM ANISOU 1819 CD ARG 266 1113 1567 1564 -17 -49 -11ARG 266 2.508 15.879 43.447 1.000 9.43 MOTA 1820 NE ANISOU 1820 NE ARG 266 1341 1157 1086 24 -100 - 145 ATOM 1821 CZ ARG 266 1.236
ANISOU 1821 CZ ARG 266 1245
ATOM 1822 NH1 ARG 266 0.961
ANISOU 1822 NH1 ARG 266 0.961
ANISOU 1823 NH2 ARG 266 0.225
ANISOU 1823 NH2 ARG 266 0.225
ANISOU 1823 NH2 ARG 266 1460
ATOM 1824 C ARG 266 6.601

1157
1006
24 -100 -14
1294
132 -159 14.567
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1.000 11.20
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191 -283 7
1870M
1824 C ARG 266 6.601
16.190
40.099
1.000 10.28 1294 132 -159 - 1 -144 -454 2 7 2 -283 7 3 266 6.601 16.190 40.099 1.000 10.28 ANISOU 1824 C ARG 1089 266 1273 1545 -200 -5 -167 1825 0 ARG 266 6.027 17.109 39.519 1.000 11.05 ANISOU 1825 O 266 1254 267 7.215 ARG 1153 1793 -132 47 - 64 ATOM 1826 N PRO 15.162 39.496 1.000 10.27 267 1194 267 7.828 ANISOU 1826 N PRO 1468 1239 -33 130 3 2 1827 CD PRO 13.963 40.109 1.000 12.36 ANISOU 1827 CD PRO 267.1865 1132 1697 -529 - 192 -26 1828 CA MOTA PRO 267 7.304 15.157 38.036 1.000 10.12 ANISOU 1828 CA PRO 267 1278 1095 1472 -129 38 - 185 ATOM 1829 CB PRO 267 8.250 13.986 37.767 1.000 11.83 ANISOU 1829 CB PRO 267 1489 1088 1919 -72 90 -32 13.053 38.913 1.000 10.72 -72 90 - 322 ATOM 1830 CG 267 8.017 PRO ANISOU 1830 CG 267 960 1356 1755 95 -257 -187 PRO

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ATOM 1831 C PRO 36		- 150 -		
11.0 20	7 5.977	14.929	37.34	4 1 000 10 06
ANISOU 1831 C PRO 26	7 1330	1226		
ATOM 1832 0 PRO 26	7 5.030		1570	-252 47 - 161
	7 1316	14.421		4 1.000 12.03
3,00%	1 7 7 7 9	1174	2080	-258 17 7 7
331TCC11 1022		15.288	36.06	5 1.000 10.61
3001 1034 -	8 1216	1146	1670	
ATOM 1834 CA ASN 26	8 4.810	14.949	35.198	
AN1300 1834 CA ASN 26	8 1285	1349		
ATOM 1835 CB ASN 26	8 4.954		1622	-167 -43 -229
ANTECOM 1005	0 4.954	15.664		5 1.000 14.02
3,000	8 2160	1410	1756	132 -316 2 3
2011	8 4.992	17.175	33.992	2 1.000 13.03
3,000	8 1811	1393	1747	= 5 . 0 5
ATOM 1837 ODI ASN 26	3 4.046	17.748	34.566	189 -355 - 88
ANISOU 183/ ODI ASN 261	3 1910	1744		
ATOM 1838 ND2 ASN 266	3 6.037		2673	292 -1 - 159
	3 2505	17.818		1.000 14.19
3,000	2505	1372	1516	161 264 - 172
ANTECOM 1000 - ADM 200	3 4.705	13.446	34.968	1.000 10.88
7 more = 0.5	3 1294	1314	1526	
ANT COTT 1040 - ASIN 208	3 5.715	12.732	34.979	
ANTIOU TO 40 U ASN 268	1534	1439		
ATUM 1841 N ATA SEC	3.484	12 000	1464	87 -458 -121
ANISOU 1841 N ALA 260	1484	12.980	34.688	
7004	7.404	1428	1732	-108 -397 - 427
ANTECOM 1040	3.277	11.547	34.417	1.000 12.12
3001	1432	1356	1819	-238 -29 -282
ANTECOM 1040 - ALIA 209	1.817	11.310	34.058	1.000 12.38
30036 1044 -	1439	1278	1985	
	4.125	10.981	33.283	-228 -183 2 9
AN1300 1844 C ALA 269	1445	1240	1500	1.000 11.26
AIUM 1845 O ATA 260	4.493	9.800	1592	25 -280 - 141
ANISOU 1845 O ALA 260	1428		33.263	1.000 12.53
ATOM 1846 N ASP 270	4.438	1249	2085	-110 108 -188
ANT COLL TO A C	4.438	11.799	32.276	1.000 11.47
70036	1701	1280	1378	-261 -341 - 300
ANTRON 1048 - ADE 2/0	5.214	11.378	31.113	1.000 11.92
7 m O 3 (10 4 0 =	1826	1106	1595	19 -183 -156
ANTICOTI TO LO ED ASP 2/0	4.760	12.096	29.850	1 000 14 13
ANISOU 1848 CB ASP 270	1733	2038	1597	1.000 14.13
ATUM 1849 CG ASP 276		13.568		84 111 2 1 2
ANISOU 1849 CG ASP 270		1939	29.777	1.000 15.98
010H 1800 OD 180 076		1939	1823	418 -418 5 6 4
ANISOU 1850 OD1 ASP 270		14.186	30.762	1.000 21.61
ATOM 1851 OD2 ACB 276		1797	2312	176 -515 1 6 3
ANT COT 1051	4.880	14.152	28.674	1.000 24.64
ATOM 1852 C ASP 270	3995	3221	2145	-62 -169 1 3 9 5
ANTICOTI 1050	6.721	11.542	31.264	1.000 12.86
30035	1840	1392	1654	-398 -61 315
ANTICOM 1050	7.443	11.290	30.292	1 000 14 03
ANT 300 1033 0 ASP 270		2114	1709	
A10M 1854 N PHF 271				-346 -141 4 9
			32.439	
ATOM 1855 CA PHE 271		1316	1824	59 - 25 7 0
ANTICOM 1055		11.927	32.715	1.000 11.14
3001	1242	1349	1641	10 230 162
· ANTCOM 1056	8.972	12.378	34.143	1.000 12.19
A TOM 1053	1467		1722	-96 -3 1 8 2 ·
ANT COULTON	10.385		34.597	1 000 10 77
11111111111111111111111111111111111111			1800	1.000 12.77
1858 CD1 PHE 271				42 31 5 6
ANISOU 1858 CD1 PHE 271	-		33.904	1.000 13.22
ATOM 1859 CD2 PHF 271			1993	168 220 4 9
		11.155	35.666	1.000 13.55
7 TOM 1000		1674	2131	139 84 2 5 5
ANTCOM 1000 - LIL FILE 2/1	12.779	12.178		1.000 14.26
	1432			-39 46 - 416
ATOM 1861 CE2 PHE 271				1.000 15 . 88
				OOO ID. 88

- 151 -ANISOU 1861 CE2 PHE 271 1537 1818 2679 -263 -675 2 6 0 1862 CZ PHE 271 13.006 11.288 35.304 1.000 14.15 ANISOU 1862 CZ 271 1166 271 9.259 PHE 1736 2475 7 -531 -467 ATOM 1863 C PHE 10.550 32.410 1.000 11.27 ANISOU 1863 C PHE 271 1359 1338 1585 75 271 3 4 8 ATOM 1864 0 PHE 271 8.785 9.531 32.920 1.000 12.97 ANISOU 1864 O 271 2011 PHE 1320 1596 -85 473 279 271 2011 1320 1596 -85 473 2 272 10.261 10.498 31.541 1.000 11.95 1865 N ATOM THR ANISOU 1865 N THR 272 1018 1503 2020 -214 300 -115 1866 CA THR 272 10.823 9.254 30.992 1.000 12.70 ANISOU 1866 CA 272 1615 THR 1557 1652 132 341 146 1867 CB MOTA 272 10.679 9.281 THR 29.450 1.000 16.79 ANISOU 1867 CB THR 272 1814 2829 1737 -595 157 -406 MOTA 1868 OG1 THR 272 9.301 9.471 29.090 1.000 18.02 ANISOU 1868 OG1 THR 272 1912 2921 2013 -497 -73 9 1 1869 CG2 THR 272 11.200 7.976 ATOM 28.856 1.000 17.02 ANISOU 1869 CG2 THR 272 2144 2857 1467 -475 538 -194 1870 C HOTA THR 272 12.272 9.057 31.423 1.000 12.02 ANISOU 1870 C THR 272 1436 1573 1559 92 603 1 3 7 ATOM 1871 0 THR 272 13.055 10.031 31.437 1.000 14.17 ANISOU 1871 O THR 272 1451 1583 2351 125 602 412 1872 N PHE 273 12.625 7.837 31.828 1.000 12.34 ANISOU 1872 N PHE 273 1402 1585 1703 17 378 158 ATOM 1873 CA PHE ANISOU 1873 CA PHE 273 13.953 7.492 32.312 1.000 12.20 273 1362 1364 1909 -126 336 147 1874 CB ATOM 273 13.951 7.514 PHE 33.861 1.000 12.37 ANISOU 1874 CB PHE 273 1362 1447 1890 -102 211 - 8 1875 CG ATOM 273 12.988 6.528 273 1398 1631 PHE 34.491 1.000 11.65 ANISOU 1875 CG PHE 1395 -367 42 -215ATOM 1876 CD1 PHE 273 11.684 6.889 34.773 1.000 14.11 ANISOU 1876 CD1 PHE 273 1531 2214 1614 -336 293 -621877 CD2 PHE 273 13.409 5.245 273 2024 1639 273 10.793 5.993 34.803 1.000 13.20 ANISOU 1877 CD2 PHE 1352 -358 339 - 9 1878 CE1 PHE 35.323 1.000 13.25 ANISOU 1878 CE1 PHE 273 1536 2081 1418 -98 447 4 2 1879 CE2 PHE 273 12.530 4.329 35.327 1.000 13.39 ANISOU 1879 CE2 PHE 273 1529 -224 140 283 1905 1654 ATOM 1880 CZ PHE 273 11.227 4.706 35.604 1.000 14.75 ANISOU 1880 CZ PHE 273 1444 2260 1902 -90 -186 2 7 5 ATOM 1881 C PHE 273 14.423 6.135 31.795 1.000 12.45 ANISOU 1881 C PHE 273 1278 1526 1927 -120 317 -31ATOM 1882 0 273 13.645 5.311 PHE 31.291 1.000 11.95 ANISOU 1882 O 273 1590 PHE 1580 1370 -137 226 ATOM 1883 N 274 15.717 5.854 SER 31.952 1.000 12.07 ANISOU 1883 N SER 274 1270 1640 1677 -29 558 MOTA 1884 CA SER 274 16.335 4.586 31.604 1.000 14.39 ANISOU 1884 CA SER 274 1583 1534 2349 43 707 3 8 4 MOTA 1885 CB SER 274 17.845 4.771 31.438 1.000 14.49 ANISOU 1885 CB SER 274 1578 1727 213 2202 695 329 ATOM 1886 OG SER 274 18.564 3.558 31.424 1.000 14.97 ANISOU 1886 OG ATOM 1887 C SER 274 1763 1848 2078 349 348 - 13SER 274 16.100 3.505 32.666 1.000 13.12 ANISOU 1887 C SER 274 1670 1481 1833 8 461 1 3.7 1888 0 ATOM 274 16.438 3.700 SER 33.834 1.000 13.50 ANISOU 1888 O 274 1493 SER 1518 2116 -65 119 1 5 ATOM 1889 N VAL 275 15.533 2.359 32.271 1.000 11.90 ANISOU 1889 N 275 1476 VAL 1618 1427 -110 490 195 ATOM 1890 CA VAL 275 15.283 1.254 33.180 1.000 11.41 ANISOU 1890 CA 275 1708 VAL 1424 1204 -8 286 7 6 1891 CB ATOM VAL 275 14.346 0.198 32.543 1.000 12.74 ANISOU 1891 CB VAL 275 1732 1300 1809 62 164 - 16

- 152 -1892 CG1 VAL 275 14.157 -1.020 33.437 1.000 16.10 ANISOU 1892 CG1 VAL 275 2352 1803 1962 -614 -663 3 7 0 1893 CG2 VAL 275 12.961 0.763 32.261 1.000 13.81 ANISOU 1893 CG2 VAL 275 1535 1786 16 363 126 1924 1894 C VAL 275 16.577 0.622 33.692 1.000 12.62 ANISOU 1894 C VAL 275 1574 1628 1594 14 375 1 3 6 1895 O MOTA VAL 275 16.729 0.405 34.926 1.000 13.01 ANISOU 1895 O VAL 275 1667 1643 1634 9 118 180 1896 N ATOM PRO 276 17.569 0.286 32.889 1.000 14.64 ANISOU 1896 N PRO 276 1583 2066 1914 2 454 - 42 1897 CD PRO 276 17.583 0.285 MOTA 31.415 1.000 15.84 ANISOU 1897 CD PRO 276 1565 2536 1916 89 755 3 5 1898 CA PRO 276 18.827 -0.250 33.453 1.000 16.76 ATOM ANISOU 1898 CA PRO 276 1667 2403 2296 261 393 - 163 1899 CB PRO 276 19.732 -0.503 32.236 1.000 18.27 ATOM ANISOU 1899 CB PRO 276 1804 2568 2571 411 574 - 142 1900 CG PRO 276 18.868 -0.385 31.029 1.000 18.96 MOTA ANISOU 1900 CG PRO 276 2147 2763 PRO 276 19.500 0.710 34.420 1.000 16.32 PRO 276 1521 2342 2336 115 237 6 PRO 276 20.035 0.277 35.456 1.000 16.78 PRO 276 1411 2689 2275 93 376 253 LEU 277 19.475 2.019 34.155 1.000 16.58 LEU 277 1835 2412 2052 -15 483 1 LEU 277 20.142 2.919 35.099 1.000 17.70 2293 725 694 - 37 1901 C ATOM ANISOU 1901 C 237 6 7 ATOM 1902 0
 276
 1411
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 277
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 ANISOU 1902 O 1903 N MOTA ANISOU 1903 N 483 148 1904 CA LEU ATOM ANISOU 1904 CA LEU 362 118 1905 CB LEU MOTA ANISOU 1905 CB LEU 1906 CG 277 21.048 5.359 ATOM LEU 35.186 1.000 20.86 277 2213 2221 277 22.446 4.888 35.53 2303 8552 ANISOU 1906 CG LEU -32 -355 4 8 2 1907 CD1 LEU 35.531 1.000 34.24 ANISOU 1907 CD1 LEU 277 2157 69 -842 2 5 8 1908 CD2 LEU 277 21.062 6.620 34.334 1.000 31.91 1908 CD2 LEU 277 4745 2460 4918 -474 -572 1 ANISOU 1908 CD2 LEU 277 4745 -474 -572 1150 1909 C LEU 277 19.411 2.989 36.430 1.000 16.55 ATOM ANISOU 1909 C LEU 277 1975 2430 1885 -218 211 -243 ATOM 1910 O LEU 277 19.997 3.116 37.517 1.000 19.19 ANISOU 1910 O LEU 277 2179 2636 2476 -617 50 1 2 -617 50 1 2 2 1911 N ALA 278 18.080 2.905 36.386 1.000 15.48 1911 N ALA 278 2008 1904 1969 -358 279 1 ATOM ANISOU 1911 N ALA 278 2008 -358 279 112 ATOM 1912 CA ALA 278 17.308 2.896 37.636 1.000 14.51
ANISOU 1912 CA ALA 278 2109 1763 1641 -309 74 167
ATOM 1913 CB ALA 278 15.814 2.896 37.347 1.000 15.41
ANISOU 1913 CB ALA 278 2017 1773 2064 66 301 6 2 6
ATOM 1914 C ALA 278 17.710 1.684 38.479 1.000 14.55
ANISOU 1914 C ALA 278 1972 1869 1689 -195 -255 7 9
ATOM 1915 O ALA 278 17.894 1.770 39.683 1.000 13.80
ANISOU 1915 O ALA 278 1444 2144 1655 -250 -166 8 9
ATOM 1916 N ARG 279 17.841 0.530 37.842 1.000 13.86
ANISOU 1916 N ARG 279 17.841 0.530 37.842 1.000 13.86
ANISOU 1916 N ARG 279 1795 1728 1742 -432 -128 169
ATOM 1917 CA ARG 279 18.242 -0.679 38.560 1.000 15.88
ANISOU 1917 CA ARG 279 18.242 -0.679 38.560 1.000 15.88
ANISOU 1918 CB ARG 279 18.204 -1.922 37.648 1.000 16.83
ANISOU 1918 CB ARG 279 1889 1897 2609 84 544 2 5 0 ATOM 1912 CA ALA 278 17.308 2.896 37.636 1.000 14.51 -432 -128 1 6 9 279 1889 1897 2609 84 544 2 5 0 279 16.790 -2.323 37.291 1.000 19.63 279 2123 2196 3139 -63 233 9 ANISOU 1918 CB ARG 1919 CG ATOM ARG ANISOU 1919 CG ARG -63 233 9 1 1920 CD ARG ANISOU 1920 CD 279 3924 ARG 3198 3150 -603 -275 - 198 -4.578 36.364 1.000 27.45 1921 NE 279 17.236 ARG ANISOU 1921 NE ARG 279 4659 -359 751 -789 2854 2915 279 16.714 -5.717 36.779 1.000 32.85 1922 CZ ARG

- 153 -ANISOU 1922 CZ ARG 279 4486 3045 4948 -475 448 -222 1923 NH1 ARG 279 15.424 -5.874 37.089 1.000 29.96 ANISOU 1923 NH1 ARG 279 4653 2168 4562 -103 967 -678 1924 NH2 ARG 279 17.551 -6.750 36.890 1.000 37.87 ANISOU 1924 NH2 ARG 279 4879 2436 -276 3278 - 824 7074 MOTA 1925 C ARG 279 19.628 -0.519 39.150 1.000 17.48 ANISOU 1925 C ARG 279 2118 1653 75 -8 7 0 5 2871 ATOM 1926 0 ARG 279 19.916 -1.064 40.212 1.000 26.82 ANISOU 1926 O ARG 279 3764 3102 3325 -1987 -1467 1383 1927 N ATOM 280 20.538 GLU 0.189 38.505 1.000 17.73 ANISOU 1927 N 280 1983 GLU 2293 2459 109 609 3 7 ATOM 1928 CA GLÜ 280 21.899 0.317 39.026 1.000 19.66 ANISOU 1928 CA GLU 280 2049 2023 3396 125 215 737 ATOM 1929 CB GLU 280 22.836 0.886 37.936 1.000 20.17 ANISOU 1929 CB GLU 280 1648 2457 3560 464 138 1099 280 22.964 ATOM 1930 CG GLU -0.149 36.818 1.000 31.79 ANISOU 1930 CG GLU 280 3477 4175 4427 801 1187 - 4 1931 CD 280 23.698 GLU 0.341 35.590 1.000 39.66 ANISOU 1931 CD GLU 280 5144 5703 4221 **-64** 1339 **-** 6 1932 OE1 GLU 280 24.466 1.327 35.685 1.000 39.65 ANISOU 1932 OE1 GLU 280 3464 5891 5710 334 574 1639 1933 OE2 GLU 280 23.489 -0.294 34.519 1.000 41.55 ATOM ANISOU 1933 OE2 GLU 280 5257 6747 2245 -184 1 0 2 3781 ATOM 1934 C GLU 280 21.984 1.188 40.266 1.000 19.68 ANISOU 1934 C GLU 280 1488 2350 3640 -566 162 490 40.958 1.000 25.69 1935 0 ATOM GLU 280 23.031 1.142 ANISOU 1935 O GLU 280 1871 3766 4123 231 -245 18 0 ATOM 1936 N CYS 281_20.943 1.980 40.565 1.000 18.57 ANISOU 1936 N CYS 281 1560 2609 2887 -406 -211 1 7 6 1937 CA CYS 281 21.098 2.762 41.806 1.000 23.83 ANISOU 1937 CA CYS 281 3222 2647 -1189 176 -122 3184 ATOM 1938 CB CYS 281 21.079 4.264 41.523 1.000 25.40 ANISOU 1938 CB CYS 281 3278 2655 3718 -426 368 - 46 MOTA 1939 SG CYS 281 19.587 4.904 40.763 1.000 27.05 ANISOU 1939 SG CYS 281 3069 2914 4295 -522 -37 -794ATOM 1940 C CYS 281 20.098 2.406 42.907 1.000 16.99 ANISOU 1940 C CYS 281 1377 1604 3475 109 -6 - 546 1941 0 ATOM CYS 281 19:971 3.173 43.889 1.000 17.04 ANISOU 1941 O CYS 281 2294 1277 2902 -204 -484 - 129 ATOM 1942 N GLY 282 19.447 1.245 42.794 1.000 15.23 ANISOU 1942 N GLY 282 1617 1597 2572 3 -58 -436 1943 CA GLY 282 18.731 43.914 1.000 15.61 0.674 ANISOU 1943 CA GLY 282 1565 1973 2394 6 -331 -266 1944 C GLY 282 17.246 0.519 43.727 1.000 13.75 ANISOU 1944 C GLY 282 1635 1562 2029 -270 -446 - 78 ATOM 1945 0 GLY 282 16.585 0.012 44.639 1.000 14.99 ANISOU 1945 O 282 1751 GLY 1630 2313 207 -242 4 5 5 ATOM 1946 N PHE 283 16.744 1.009 42.582 1.000 12.65 ANISOU 1946 N PHE 283 1434 1803 1570 -200 18 - 252 ATOM 1947 CA PHE 283 15.292 0.886 42.374 1.000 11.80 ANISOU 1947 CA PHE 283 1477 1032 -264 4 6 1974 -15 1948 CB ATOM PHE 283 14.839 1.890 41.295 1.000 14.13 ANISOU 1948 CB PHE 283 2262 972 2136 109 -187 159 1949 CG MOTA 283 14.906 PHE 3.351 41.757 1.000 12.63 ANISOU 1949 CG PHE 283 1711 1033 2055 47 -86 9 1950 CD1 PHE ATOM 283 13.851 3.928 42.409 1.000 13.45 ANISOU 1950 CD1 PHE 283 1697 1399 2013 -166 24 - 229 ATOM 1951 CD2 PHE 283 16.037 4.111 41.519 1.000 13.15 ANISOU 1951 CD2 PHE 283 1567 1135 2295 142 -41 - 9 9 1952 CE1 PHE 283 13.903 5.248 42.839 1.000 15.61 ANISOU 1952 CE1 PHE 283 2111 1649 2171 -202 484 -617

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1953 CE2 PHE 283 16.112 5.432 41.963 1.000 12.60 1953 CE2 PHE 283 1783 937 2068 32 -18 264 1954 CZ PHE 283 15.040 5.993 42.641 1.000 13.37 1954 CZ PHE 283 1863 865 2352 187 -149 1 3 1955 C PHE 283 14.915 -0.534 41.972 1.000 11.23 1955 C PHE 283 1527 974 1765 63 -172 6 5 1956 O PHE 283 15.471 -1.071 40.990 1.000 13.24
     ANISOU 1953 CE2 PHE
     ANISOU 1954 CZ
  ATOM 1955 C PHE 283 14.915 -0.534 41.972 1.000 11.23
ANISOU 1956 O PHE 283 15.471 -1.071 40.990 1.000 13.24
ANISOU 1956 O PHE 283 1249 1428 2355 175 -120 - 36.2
ATOM 1957 N ASP 284 13.998 -1.130 42.712 1.000 12.31
ANISOU 1957 N ASP 284 1607 1333 1736 -268 -312 8 7
ANISOU 1958 CA ASP 284 13.589 -2.528 42.527 1.000 12.48
ATOM 1959 CB ASP 284 1725 1202 1814 -148 -543 3 5 0
ANISOU 1959 CB ASP 284 13.159 -3.156 43.876 1.000 12.67
ANISOU 1959 CB ASP 284 2014 1145 1656 -50 -406 1 3 5
ANISOU 1960 CG ASP 284 13.261 -4.667 43.909 1.000 13.40
ANISOU 1960 CG ASP 284 2077 1171 1843 110 -419 3 6 3
ATOM 1961 OD1 ASP 284 13.861 -5.246 42.974 1.000 1 4.98
     ATOM
                                                                                                                                                                                           175 -120 - 361
                              1961 OD1 ASP 284 13.861 -5.246 42.974 1.00(14.98
   ANISOU 1961 OD1 ASP 284 1956 1094 2640 -87 11 6 0
ATOM 1962 OD2 ASP 284 12.762 -5.306 44.883 1.000 15.79
ANISOU 1962 OD2 ASP 284 2494 1539 1966 -330 -446 4
  ANISOU 1962 OD2 ASP 284 2494 1539 1966 -330 -446 43 ATOM 1963 C ASP 284 12.478 -2.641 41.510 1.000 10.82 ATOM 1964 O ASP 284 1238 1387 1487 -205 -99 12 ANISOU 1964 O ASP 284 11.373 -3.100 41.777 1.000 12.28 ATOM 1965 N VAL 285 12.751 -2.154 40.308 1.000 11.32 ANISOU 1965 N VAL 285 12.751 -2.154 40.308 1.000 11.32 ATOM 1966 CA VAL 285 1204 1671 1426 -93 -48 6 1 ANISOU 1966 CA VAL 285 1468 1384 1500 39 -219 -15 ATOM 1967 CB VAL 285 1468 1384 1500 39 -219 -15
                                                                                                                                                                                            -330 -446438
                                                                                                                                                                                           -205 -99 123
ANISOU 1965 N VAL 285 1204 1071 1420

ATOM 1966 CA VAL 285 11.748 -2.062 39.260 1.000 11.45

ANISOU 1966 CA VAL 285 1468 1384 1500 39 -219 - 15

ATOM 1967 CB VAL 285 12.153 -1.072 38.157 1.000 11.58

ATOM 1968 CG1 VAL 285 1412 1523 1465 -388 -428 - 8

ATOM 1968 CG1 VAL 285 12.278 0.362 38.679 1.000 15.02

ANISOU 1968 CG1 VAL 285 2209 1458 2040 -264 -442 - 32

ANISOU 1969 CG2 VAL 285 13.467 -1.482 37.495 1.000 15.70

ANISOU 1969 CG2 VAL 285 1909 1443 2615 -159 309 447

ATOM 1970 C VAL 285 1909 1443 2615 -159 309 447

ATOM 1970 C VAL 285 1224 38.642 1.000 10.83

ANISOU 1970 C VAL 285 1232 1281 1602 93 -221 108

ATOM 1971 O VAL 285 12267 -4.301 38.520 1.000 12.13

ANISOU 1971 O VAL 285 1214 1192 2202 -28 300 162

ATOM 1972 N SER 286 10.168 -3.523 38.248 1.000 11.09

ANISOU 1973 CA SER 286 9.558 -4.622 37.510 1.000 11.32

ATOM 1973 CA SER 286 1116 1608 1489 -76 96 7

ATOM 1973 CA SER 286 9.558 -4.622 37.510 1.000 11.32

ATOM 1974 CB SER 286 8.483 -5.292 38.344 1.000 9.88

ANISOU 1974 CB SER 286 1328 1141 1285 72 -207 7 0

ANISOU 1975 OG SER 286 7.570 -4.361 38.905 1.000 11.34
 ATOM 1974 CB SER 286 8.483 -5.292 38.344 1.000 9.88 ANISOU 1974 CB SER 286 1328 1141 1285 72 -207 7 0 ANISOU 1975 OG SER 286 7.570 -4.361 38.905 1.000 11.34 ATOM 1976 C SER 286 9.019 -4.106 36.175 1.000 10.34 ATOM 1976 C SER 286 9.019 -4.106 36.175 1.000 10.34 ATOM 1977 O SER 286 7.829 -4.112 35.869 1.000 12.62 ANISOU 1977 O SER 286 1223 2219 1353 0 -178 228 ANISOU 1978 N LEU 287 9.926 -3.622 35.335 1.000 12.45 ANISOU 1978 N LEU 287 1414 1664 1653 -212 3 161
  ANISOU 1978 N
                                                                                   LEU
                                                                                                                                                                                           -212 3 161
                             1979 CA
                                                             LEU
  ANISOU 1979 CA
                                                             LEU
                                                                                    287 1622 1558 1605 -366 94 184
287 10.145 -1.452 34.210 1.000 12.91
                                                                                                                                                                                           -366 94 184
  ATOM
                             1980 CB
                                                              LEU
  ANISOU 1980 CB
                                                                                    287 1716
287 9.452
                                                              LEU
                                                                                                                                 1591
                                                                                                                                                            1597
                                                                                                                                                                                           -373 -95 2 7
  MOTA
                             1981 CG
                                                              LEU
                                                                                                                            -0.590 35.264 1.000 12.96
                                                                                   ANISOU 1981 CG LEU
                                                                                                                                                                                           -407 -51 -170
                           1982 CD1 LEU
  ANISOU 1982 CD1 LEU
                                                                                                                                                              2318 -38 -124 2 2 3
                            1983 CD2 LEU 287 8.006
  ATOM
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- 155 -

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1983 CD2 LEU 287 1716 1548 2267 36 -550 318 1984 C LEU 287 10.319 -3.610 32.928 1.000 12.63
      ANISCU 1983 CD2 LEU 287 1716
                                                                                                                                                                                                                                                                                 36 -550 318
    ATOM 1998 N GLU 290 13.562 -0.952 27.869 1.000 16.48
ANISOU 1998 N GLU 290 2665 2099 1496 5 222 -445
   ATOM 1999 CA GLU 290 14.716 -0.117 28.182 1.000 16.94

ANISOU 1999 CA GLU 290 2470 2161 1806 81 411 -484

ATOM 2000 CB GLU 290 15.579 0.012 26.912 1.000 20.26

ANISOU 2000 CB GLU 290 2670 2740 2287 414 863 -1
ATOM 2000 CB GLU 290 15.579 0.012 26.912 1.000 20.26 ANISOU 2000 CB GLU 290 2670 2740 2287 414 863 -239 ATOM 2001 CG GLU 290 16.071 -1.333 26.386 1.000 24.53 ANISOU 2001 CG GLU 290 3251 3153 2916 664 1218 -612 ATOM 2002 CD GLU 290 3019 3161 4424 989 940 -251 ATOM 2002 CD GLU 290 3019 3161 4424 989 940 -251 ATOM 2003 OE1 GLU 290 17.874 -1.747 27.917 1.000 35.13 ANISOU 2003 OE1 GLU 290 3913 4458 4975 963 -85 -877 ATOM 2004 OE2 GLU 290 16.336 -3.280 27.734 1.000 43.76 ANISOU 2004 OE2 GLU 290 6893 3257 6478 -30 -748 598 ATOM 2005 C GLU 290 6893 3257 6478 -30 -748 598 ATOM 2005 C GLU 290 2512 1756 1308 95 142 1 0 ANISOU 2005 C GLU 290 2512 1756 1308 95 142 1 0 ANISOU 2006 O GLU 290 2512 1756 1308 95 142 1 0 ANISOU 2006 O GLU 290 2512 1756 1308 95 142 1 0 ANISOU 2007 N THR 291 13.232 1.814 28.437 1.000 15.25 ANISOU 2007 N THR 291 13.232 1.814 28.437 1.000 15.72 ANISOU 2008 CA THR 291 12.792 3.087 28.991 1.000 15.16 ANISOU 2009 CB THR 291 12.766 4.226 27.956 1.000 18.67 ANISOU 2009 CB THR 291 12.766 4.226 27.956 1.000 18.67 ANISOU 2009 CB THR 291 12.766 4.226 27.956 1.000 18.67 ANISOU 2010 OG1 THR 291 11.756 4.009 26.976 1.000 22.93 ANISOU 2010 OG1 THR 291 11.756 4.009 26.976 1.000 22.93 ANISOU 2010 CG2 THR 291 14.096 4.306 27.213 1.000 21.82 ATOM 2011 CG2 THR 291 14.096 4.306 27.213 1.000 12.86 ATOM 2012 C THR 291 1863 1604 1421 47 305 21 9 ATOM 2012 C THR 291 1863 1604 1421 47 305 21 9 ATOM 2013 O THR 291 1863 1604 1421 47 305 21 9 ATOM 2013 O THR 291 1863 1604 1421 47 305 21 9 ATOM 2013 O THR 291 1863 1604 1421 47 305 21 9 ATOM 2013 O THR 291 11.602 2.920 2.024 2.024 2.024 2.024 2.026 2.024 2.026 2.024 2.026 2.024 2.026 2.024 2.026 2.024 2.026 2.024 2.026 2.024 2.026 2.024 2.026 2.024 2.026 2.024 2.026 2.026 2.024 2.026 2.026 2.024 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 2.026 
                                                                                             THR 291 1863 1604 1421 47 305 219
THR 291 10.625 2.024 29.270 1.000 16.13
    MOTA
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    ANISOU 2013 O
                                                                                             THR 291 2344 1983 1804 -303 750 -431
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- 156 -MOTA 2014 N ALA 292 11.037 3.791 30.542 1.000 12.41 ANISOU 2014 N ALA 292 1495 1363 -2 256 7 7 1859 2015 CA ALA 292 9.746 31.202 1.000 11.57 3.839 ANISOU 2015 CA ALA 292 1362 1257 1779 -213 153 3 7 ALA 292 9.718 2.954 ALA 292 1768 1245 ALA 292 9.385 5.255 ALA 292 1317 1335 2016 CB 32.439 1.000 12.62 ANISOU 2016 CB ALA 292 1768 1784 100 357 2017 C 31.614 1.000 10.32 ANISOU 2017 C 1270 -181 99 5 4 ALA 292 10.266 6.134 2018 0 MOTA 31.701 1.000 10.97 ANISOU 2018 O ALA 292 1389 1138 1641 -146 279 104 THR 293 8.091 5.445 THR 293 1486 1547 2019 N MOTA 31.882 1.000 12.32 ANISOU 2019 N 1647 -314 563 -284 THR 293 7.626 6.715 32.421 1.000 12.28 THR 293 1717 1460 1489 -168 337 -2020 CA MOTA ANISOU 2020 CA ATOM 2021 CB THR 293 6.352 7.215 31.733 1.000 13.27 ANISOU 2021 CB THR 293 2128 1182 1730 -258 -159 -ATOM 2022 OG1 THR 293 5.317 6.237 31.911 1.000 13.85 ANISOU 2022 OG1 THR 293 1831 1217 2216 8 -131 7 4 -168 337 - 200-258 -159 - 284 ATOM 2023 CG2 THR 293 6.474 7.303 30.212 1.000 13.72 ANISOU 2023 CG2 THR 293 1791 1683 1738 -252 -56 --252 -56 -405 THR 293 7.363 6.635 33.937 1.000 10.58 THR 293 1439 1050 1533 12 447 9 ATOM 2024 C THR 293 1439 1050 1533 12 447 9
THR 293 7.211 5.576 34.553 1.000 10.29
THR 293 1049 1102 1758 -56 93 1 1 8
PHE 294 7.243 7.810 34.569 1.000 11.53
PHE 294 1794 1093 1494 -307 306 -66
PHE 294 6.806 7.939 35.950 1.000 10.41
PHE 294 1432 1061 1463 -174 125 -162
PHE 294 6.709 9.426 36.336 1.000 12.25
PHE 294 1930 1030 1694 -164 292 -64
PHE 294 6.270 9.658 37.770 1.000 12.77
PHE 294 1880 1136 1837 -103 178 -427
PHE 294 7.123 9.462 38.839 1.000 14.73
PHE 294 1976 1893 1727 -539 161 -132
PHE 294 4.989 10.068 38.056 1.000 16.59
PHE 294 2180 1923 2199 348 386 -492
PHE 294 6.726 9.673 40.144 1.000 14.36
PHE 294 1598 2028 1830 -505 280 -118 ANISOU 2024 C ATOM 2025 0 ANISOU 2025 O 2026 N ATOM ANISOU 2026 N ATOM 2027 CA ANISOU 2027 CA 2028 CB ANISOU 2028 CB 2029 CG ANISOU 2029 CG PHE 2030 CD1 PHE ANISOU 2030 CD1 PHE ATOM 2031 CD2 PHE ANISOU 2031 CD2 PHE ATOM 2032 CE1 PHE ANISOU 2032 CE1 PHE 294 1598 2028 1830 -505 280 -294 4.575 10.275 39.345 1.000 16.75 1830 -505 280 -118 2033 CE2 PHE ATOM ANISOU 2033 CE2 PHE 294 2214 2062 2087 692 144 - 602 294 5.426 10.065 40.413 1.000 15.17 ATOM 2034 CZ PHE ANISOU 2034 CZ PHE 327 97 - 135 2035 C ATOM PHE ANISOU 2035 C PHE PHE 294 1401 1200 1536 -155 78 13 PHE 294 5.325 6.425 37.125 1.000 10.67 -155 78 1 3 7 MOTA 2036 0 ANISOU 2036 O PHE 294 1396 1297 1360 90 337 1 0 5 ATOM 2037 N ANISOU 2037 N GLN 295 4.487 7.355 35.299 1.000 10.62 GLN 295 1399 1187 1450 -18 88 - 24 ATOM 2038 CA GLN 295 3.217 6.612 35.393 1.000 11.31 ANISOU 2038 CA GLN 295 1433 1205 1660 -96 120 -321 ATOM 2039 CB 295 2.284 7.053 34.254 1.000 11.66 ATOM 2039 CB GLN 295 2.284 7.053 34.254 1.000 11.66
ANISOU 2039 CB GLN 295 1425 1053 1953 -25 63 -14
ATOM 2040 CG GLN 295 0.951 6.360 34.200 1.000 11.05
ANISOU 2040 CG GLN 295 1573 1011 1614 -93 -118 1
ATOM 2041 CD GLN 295 0.052 6.843 33.087 1.000 11.35
ANISOU 2041 CD GLN 295 1592 1326 1395 173 57 - 13
ATOM 2042 OE1 GLN 295 0.349 7.823 32.378 1.000 15.06
ANISOU 2042 OE1 GLN 295 2306 1589 1825 110 7 3 7 9
ATOM 2043 NE2 GLN 295 -1.053 6.153 32.914 1.000 13.90
ANISOU 2043 NE2 GLN 295 1511 1757 2015 156 -282 2
ATOM 2044 C GLN 295 3.412 5.107 35.389 1.000 10.12 GLN -25 63 - 141 -93 -118 1 8 57 - 13156 -282 2 0 8

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ANISOU	2011	\sim	CIN	20-	1151			
			GLN		1154	1203	1486	21 160 - 191
MOTA	2045		GLN		2.827	4.309	36.128	1.000 11.82
ANISOU			GLN	295	1264	1542	1686	-107 41 1 3 7
ATOM	2046	N	ASP		4.267	4.558	34.538	1.000 9 . 3 5
ANISOU			ASP	_				
					1076	1056	1422	-118 -76 -275
ATOM	2047		ASP		4.655	3.172	34.416	1.000 9 . 9 1
ANISOU	2047	CA	ASP	296	1241	1139	1387	56 60 - 243
ATOM	2048	CB	ASP		5.699	2.852	33.347	1.000 10.26
ANISOU			ASP		1315	1156		
ATOM	2049						1429	113 132 - 36
			ASP		5.343	2.981	31.885	1.000 11.42
ANISOU			ASP		1357	1578	1405	358 121 - 199
ATOM	2050	OD1	ASP	296	4.143	2.904	31.531	1.000 13.82
ANISOU	2050	OD1	ASP		1511	1744	1997	149 -209 - 62
ATOM	2051				6.282			
ANISOU	2051	000	ACD			3.151	31.047	1.000 13.48
					1802	1758	1564	228 364 7 3
MOTA	2052	С	ASP		5.175	2.682	35.770	1.000 10.31
ANISOU	2052	C	ASP	296	1416	1141	1361	16 91 - 198
MOTA	2053	j	ASP		4.852	1.551	36.197	1.000 11.40
ANISOU			ASP		1428			
	2054					1452	1453	-288 32 3 5
ATOM			TRP	297	6.004	3.484	36.441	1.000 10.88
ANISOU		N	TRP		1752	1144	1238	-161 11 5 5
ATOM	2055	CA	TRP	297	6.646	3.104	37.685	1.000 11.26
ANISOU	2055	CA	TRP	297	1768	1215	1294	-217 -57 4 5
ATOM	2056	СВ	TRP	297	7.899			
ANISOU						3.999	37.890	1.000 10.31
			TRP		1387	1417	1112	-87 213 120
ATOM	2057		TRP		8.621	3.651	39.172	1.000 10.98
ANISOU	2057	CG	TRP	297	1456	1394	1324	164 -29 - 43
ATOM	2058	CD2	TRP		9.082	4.534	40.202	1.000 12.49
ANISOU			TRP	297	1255	1729	1761	
ATOM	2059							75 - 298 - 197
					9.692	3.755	41.201	1.000 16.08
ANISOU			TRP		1860	2049	2202	-294 -977 4 9
\mathtt{ATOM}	2060	CE3		297	9.040	5.910	40.379	1.000 17.41
ANISOU	2060	CE3	TRP		2778	1740	2096	-388 -916 - 234
ATOM	2061			297		2.400	39.589	
ANISOU	2061	CDI	UD D					1.000 13.58
	2001	CDI	IRP		1617	1518	2025	0 -664 114
MOTA	2062	NET	TRP		9.614	2.444	40.808	1.000 16.12
UOZINA		NE1	\mathtt{TRP}	297	2165	1909	2051	-22 -873 2 2 0
\mathtt{ATOM}	2063	CZ2	TRP	297	10.243	4.320	42.341	1.000 19.85
ANISOU	2063	CZ2			2756	2383	2404	
ATOM	2064		TRP		9.586			
ANISOU			TAP			6.466	41.515	1.000 23.40
	2004	C Z 3	TRP	297	4215	2030	2645	-1001 -1757 - 77
ATOM	2065	CH2	TRP	297	10.181	5.670	42.486	1.000 21.51
ANISOU	2065	CH2	TRP	297	3178	2457	2537	-910 -1473 - 51
ATOM	2066		TRP		5.700	3.138	38.882	1.000 10.39
ANISOU			TRP		1172			
ATOM	2067			207	11/2	1448	1329	-280 -237 3 9 1
	2007	0	TRP	29/	5.574	2.159	39.639	1.000 13.52
ANISOU			TRP		1748	1830	1557	32 -91 7 0 3
MOTA	2068	N	ILE	298	5.033	4.272	39.079	1.000 12.08
ANISOU	2068	N	ILE		1400	1710	1480	-49 83 4 5 1
ATOM	2069		ILE		4.223	4.521		
ANISOU							40.272	1.000 13.43
			ILE		1301	2484	1317	-199 -158 - 3 3
ATOM	2070		ILE		4.370	5.988	.40.689	1.000 16.97
ANISOU			ILE	298	1877	2908	1661	-1000 214 -630
ATOM	2071	CG2	ILE		3.538	6.423	41.876	1.000 22.01
ANISOU	2071	CG2	TT.F	200	3980	3121		
ATOM	2072	001	TIP				1263	-233 546 -339
	2012	C G T	T 7 T		5.847	5.253	41.037	1.000 27.10
ANISOU	20/2	CGI	TLE		2588	5151	2557	-2140 -708 9 7
ATOM	2073	CDI	ILE	298	6.365	5.522	42.266	1.000 43.13
ANISOU	2073	CD1	ILE		5185	8299	2904	-3717 -3055 7 0 8
ATOM	2074	C	ILE		2.772	4.116	40.131	
ANISOU			ILE					1.000 10.94
	2014	_	ナルロ	278	1350	1652	1156	-165 -79 9 6

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- 158 -
                                                                                           ILE 298 2.137 3.844 41.155 1.000 12.67 ILE 298 1689 1634 1493 -102 212 352 GLY 299 1412 1057 1384 -51 -377 201 GLY 299 0.866 3.822 38.695 1.000 10.72 GLY 299 1335 1084 1655 0 -2229 -206
           ATOM
                                                2075 O
           ANISCU 2075 O
           MOTA
                                                2076 N
          ANISOU 2076 N
         MOTA
                                               2077 CA
                                                                                                                  299 0.866 3.822 38.695 1.000 10.72

299 1335 1084 1655 0 -229 -206

299 0.049 5.054 38.369 1.000 12.05

299 1422 1293 1864 105 -292 0

299 0.585 6.088 37.976 1.000 13.11

300 -1.268 4.931 38.490 1.000 13.92

300 1393 1531 2363 182 -410 -223

300 2.237 5.932 38.087 1.000 14.02

300 1524 1471 2331 217 -563 -336

300 -2.587 7.015 39.074 1.000 11.97

300 940 1603 2004 67 -488 -295

300 -3.322 7.950 38.722 1.000 10.90
          ANISOU 2077 CA
          ATOM
                                               2078 C
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          ANISOU 2078 C
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          ANISOU 2079 O
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         ATOM
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         ANISOU 2080 N
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        ATOM
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        ANISOU 2081 CA GLY
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        ANISOU 2083 O
                                                                                         GLY 300 1219 1408 1515 -37 -203 - 134
ASN 301 -2.090 6.910 40.285 1.000 11.64
   ATOM 2084 N ASN 301 -2.090 6.910 40.285 1.000 11.64
ANISOU 2084 N ASN 301 948 1557 1917 -383 -327 165
ANISOU 2085 CA ASN 301 -2.195 7.915 41.323 1.000 13.39
ATOM 2086 CB ASN 301 1626 1904 1557 -191 -403 18
ANISOU 2086 CB ASN 301 -3.047 7.301 42.427 1.000 17.60
ATOM 2087 CG ASN 301 1391 2869 2426 -9 326 2 2 8
ANISOU 2087 CG ASN 301 -4.021 8.196 43.108 1.000 19.15
ATOM 2088 OD1 ASN 301 -5.072 8.606 42.591 1.000 15.47
ANISOU 2088 OD1 ASN 301 1258 2340 2280 -253 339 - 8
ANISOU 2089 ND2 ASN 301 -3.661 8.510 44.367 1.000 29.28
ANISOU 2089 ND2 ASN 301 3585 4783 2758 1521 -850 -8
ATOM 2090 C ASN 301 -0.862 8.331 41.914 1.000 11.31
       ATOM
                                            2084 N
                                                                                                                                                                                                                                                                      -191 -403 183
                                                                                                                                                                                                                                                                      -253 339 - 8
 ANISOU 2089 ND2 ASN 301 3585 4783 2758 1521 -850 -88 ATOM 2090 C ASN 301 1436 1669 1194 1 1 -168 ANISOU 2091 O ASN 301 1483 1548 1542 -151 -279 8 2 ANISOU 2092 N TYR 302 -0.634 ANISOU 2092 N TYR 302 1186 1584 16611 -61 26 10 2 ANISOU 2093 CA TYR 302 0.573 ANISOU 2094 CB TYR 302 1260 ANISOU 2094 CB TYR 302 1260 ANISOU 2094 CB TYR 302 1260 ANISOU 2095 CG TYR 302 1768 ANISOU 2095 CG TYR 302 1768 ANISOU 2095 CG TYR 302 1385 ANISOU 2096 CD1 TYR 302 1385 ANISOU 2096 CD1 TYR 302 2.421 ANISOU 2096 CD1 TYR 302 2.859 ANISOU 2097 CE1 TYR 302 2.859 ANISOU 2097 CE1 TYR 302 1055 ANISOU 2098 CD2 TYR 302 1055 ANISOU 2097 CE1 TYR 302 2050 ANISOU 2097 CE1 TYR 302 
                                                                                                                                                                                                                                                                        1521 -850 -885
ANISOU 2097 CE1 TYR
                                                                                                                  302 1055 1241 1732 -11 52 - 1
302 0.161 12.793 40.858 1.000 11.30
   MOTA
                                       2098 CD2 TYR
  ANISOU 2098 CD2 TYR
                                                                                                                  302 1304 1332 1656 -145 105 - 26
302 0.573 13.406 39.690 1.000 11.72
                                      2099 CE2 TYR
  ANISOU 2099 CE2 TYR
                                                                                                              302 1013

302 1097

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                                       2100 CZ TYR
  ANISOU 2100 CZ
                                                                                     TYR
                                      2101 OH TYR
  ATOM
 ANISOU 2101 OH TYR
                                                                                                              302 1192 1532 1766 -8 102 1 0 4
302 0.654 9.349 44.196 1.000 12.45
  ATOM
                                       2102 C
                                                                                     TYR
  ANISOU 2102 C
                                                                                     TYR
                                                                                                              302 1517 1450 1765 -181 -202 2 1
302 -0.375 9.230 44.878 1.000 13.55
                                                                                                                                                                                                                                                                   -181 -202 2 1 7
 ATOM
                                      2103 0
                                                                                    TYR
 ANISOU 2103 O
                             U 2103 O TYR 302 1464 1925 1759 -339 -211 7
2104 N VAL 303 1.868 8.967 44.542 1.000 12.06
2105 CA VAL 303 2.309 8.430 45.820 1.000 11.88
 MOTA
ANISOU 2104 N
                                                                                                                                                                                                                                                                    -135 -3 3 4 0
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- 159 -ANISOU 2105 CA VAL 303 1434 1609 1471 -368 -197 2 2 ATOM 2106 CB VAL 303 2.755 6.967 45.736 1.000 14.57 ANISOU 2106 CB VAL 303 1395 1682 2459 -217 -918 3 1 ATOM 2107 CG1 VAL 303 3.131 6.462 47.132 1.000 17.33 ANISOU 2107 CG1 VAL 303 2644 1608 2331 -48 -1114 6 ATOM 2108 CG2 VAL 303 1.703 6.041 45.122 1.000 14.80 ANISOU 2108 CG2 VAL 303 1876 1676 2069 -592 -639 3 2 -368 -197 2 2 3 2459 -217 -918 3 1 2 -48 -1114 6 1 2109 C ATOM ANISOU 2109 C 2110 0 ATOM ANISOU 2110 O -61 323 -999 2111 N MOTA ANISOU 2111 N 2112 CA ASN MOTA ANISOU 2112 CA ASN 2113 CB ASN MOTA ANISOU 2113 CB ASN 2114 CG ATOM ANISOU 2114 CG ASN 2115 OD1 ASN ANISOU 2115 OD1 ASN 2116 ND2 ASN ANISOU 2116 ND2 ASN 304 1414 2117 C ANISOU 2117 C ATOM 2118 O ASN 304 1382 1299 1566 -183 -163 1 ANISOU 2118 O ASN 304 6.396 11.232 48.699 1.000 12.07 ANISOU 2119 N ILE 305 5.092 9.541 49.516 1.000 12.56 ANISOU 2119 N ILE 305 1791 1296 1685 -152 -232 2 -167 -66 -59 ATOM 2119 N ILE 305 5.092 9.541 49.516 1.000 12.56 ANISOU 2119 N ILE 305 1791 1296 1685 -152 -232 2 0 2 ATOM 2120 CA ILE 305 6.063 9.011 50.463 1.000 14.01 ANISOU 2121 CB ILE 305 5.781 9.493 1614 -55 -479 7 9 ATOM 2121 CB ILE 305 5.781 9.493 51.906 1.000 14.44 ANISOU 2121 CB ILE 305 5.781 9.493 51.906 1.000 14.44 ANISOU 2121 CG2 ILE 305 5.725 11.017 51.956 1.000 15.31 ANISOU 2122 CG2 ILE 305 1768 1608 2441 43 -479 -314 ANISOU 2123 CG1 ILE 305 1768 1608 2441 43 -479 -314 ANISOU 2123 CG1 ILE 305 1779 1694 2163 27 -307 -153 ANISOU 2124 CD1 ILE 305 4.163 9.252 53.900 1.000 28.68 ANISOU 2124 CD1 ILE 305 4.163 9.252 53.900 1.000 28.68 ANISOU 2125 C ILE 305 6.059 7.487 50.389 1.000 12.79 ANISOU 2125 C ILE 305 6.059 7.487 50.389 1.000 12.79 ANISOU 2126 O ILE 305 5.111 6.864 49.897 1.000 15.63 ATOM 2126 O ILE 305 5.111 6.864 49.897 1.000 15.63 ANISOU 2127 N ARG 306 7.170 6.896 50.829 1.000 13.04 ANISOU 2128 CA ARG 306 7.340 ANISOU 2128 CA ARG 306 1352 1366 1773 -375 -154 4 4 4 ANISOU 2129 CB ARG 306 1352 1366 1773 -375 -154 4 4 4 ANISOU 2129 CB ARG 306 1352 1366 1773 -375 -154 4 4 4 ANISOU 2129 CB ARG 306 8.203 ANISOU 2130 CG ARG 306 2566 1953 2001 -68 -68 7 6 ATOM 2131 CD ARG 306 2566 1953 2001 -68 -68 7 6 ATOM 2131 CD ARG 306 2921 2361 2130 -397 -396 -302 ATOM 2131 CD ARG 306 2921 2361 2130 -397 -396 -302 ATOM 2131 CD ARG 306 7.078 3.198 47.212 1.000 20.655 -152 -232 2 0 2 2131 CD ARG 306 8.344 3.075 47.937 1.000 19.51 2131 CD ARG 306 2921 2361 2130 -397 -396 -3 2132 NE ARG 306 7.078 3.198 47.212 1.000 20.65 2132 NE ARG 306 2693 2844 2309 -1056 -310 21 2133 CZ ARG 306 6.948 3.186 45.893 1.000 17.11 2133 CZ ARG 306 2006 2225 2268 45 -91 5 9 6 2134 NH1 ARG 306 8.013 3.065 45.083 1.000 21.58 2134 NH1 ARG 306 2405 2677 3116 -232 381 -6 2135 NH2 ARG 306 5.734 3.301 45.365 1.000 17.51 2135 NH2 ARG 306 2235 1550 2868 150 -484 -1 ANISOU 2131 CD ARG 306 2921 2130 -397 -396 - 302 ATOM ANISOU 2132 NE ARG 306 2693 -1056 -310 2 1 4 MOTA ANISOU 2133 CZ ARG ANISOU 2134 NH1 ARG 3116 -232 381 -669 ANISOU 2135 NH2 ARG -484 - 162

- 161 -ANISOU 2166 02 AKG 313 2407 1765 2587 74 - 377 429 2167 C2 MOTA AKG 313 6.867 15.178 55.844 1.000 20.08 ANISOU 2167 C2 AKG 313 1997 2566 3068 -528 419 -399 2168 05 ATOM AKG 313 7.982 14.661 55.821 1.000 17.60 ANISOU 2168 05 AKG 313 2289 2066 2334 -314 226 -252 MOTA 2169 C3 16.080 56.872 1.000 21.69 AKG 313 6.272 ANISOU 2169 C3 AKG 313 2751 1910 3581 240 62 - 3272170 C4 ATOM AKG 313 7.318 16.741 57.716 1.000 21.50 ANISOU 2170 C4 AKG 313 3246 1761 3160 199 -143 - 185ATOM 2171 C5 AKG 17.816 58.672 1.000 22.58 313 6.923 ANISOU 2171 C5 AKG 313 3122 1840 3618 755 -495 - 3132172 03 ATOM AKG 313 7.754 18.591 59.124 1.000 27.48 ANISOU 2172 03. AKG 313 3581 2470 4389 -34 602 -1266 ATOM 2173 04 AKG 313 5.660 17.889 58.999 1.000 28.55 ANISOU 2173 04 AKG 313 3191 2809 4846 612 -246 -1148 MOTA 2174 S SO4 401 11.676 0.439 24.942 1.000 40.14 2175 01 ATOM SO4 401 11.293 0.826 26.321 1.000 33.12 2176 02 ATOM SO4 401 12.501 -0.829 25.014 1.000 35.79 2177 03 ATOM SO4 401 10.430 0.189 24.129 1.000 54.89 ATOM 2178 04 SO4 401 12.500 1.520 24.329 1.000 44.80 2179 OW ATOM нон 501 ~6.455 10.219 44.319 1.000 14.29 2180 OW ATOM HOH 502 -10.520 18.612 50.560 1.000 12.86 ATOM 2181 OW нон 503 -8.644 16.907 47.858 1.000 16.83 MOTA 2182 OW HOH 504 -10.313 20.800 43.074 1.000 16.10 ATOM 2183 OW HOH 505 -6.051 19.199 52.602 1.000 16.38 MOTA 2184 OW HOH 506 -6.873 24.642 47.100 1.000 20.55 ATOM 2185 OW НОН 507 10.676 -4.179 46.406 1.000 27.41 ATOM 2186 OW 21.786 40.872 1.000 15.22 нон 508 -0.077 ATOM 2187 OW HOH 509 5.761 13.656 46.041 1.000 17.40 MOTA 2188 OW HOH 510 29.135 51.982 1.000 18.40 52.741 1.000 17.03 31.449 2189 OW ATOM НОН 511 26.032 32.724 MOTA 2190 OW HOH 512 10.965 32.371 46.000 1.000 16.70 2191 OW ATOM HOH 513 23.871 24.457 58.649 1.000 18.71 2192 OW MOTA HOH 514 26.353 29.063 50.326 1.000 18.96 2193 OW ATOM HOH515 23.191 33.106 53.153 1.000 20.41 ATOM 2194 OW HOH 516 21.429 11.721 55.329 1.000 18.39 2195 OW ATOM HOH 517 9.122 15.567 53.585 1.000 24.87 2196 OW MOTA HOH 518 27.843 17.352 53.437 1.000 27.76 2197 OW ATOM HOH519 -14.415 20.029 44.444 1.000 23.47 MOTA 2198 OW HOH 520 15.253 33.050 51.771 1.000 27.20 ATOM 2199 OW HOH 521 14.080 31.486 44.302 1.000 21.58 ATOM 2200 OW нон 522 17.770 33.842 53.596 1.000 23.56 ATOM 2201 OW 523 3.671 HOH 36.173 1.000 20.95 24.673 ATOM 2202 OW HOH 524 -15.683 28.618 52.535 1.000 24.05 ATOM нон 2203 OW 525 -5.386 20.413 39.013 1.000 26.85 ATOM 2204 OW НОН 526 10.417 27.949 58.778 1.000 28.33 ATOM 2205 OW HOH 527 23.165 19.592 62.202 1.000 29.36 ATOM 2206 OW HOH 528 23.736 10.550 55.737 1.000 24.02 ATOM 2207 OW 529 -1.662 28.650 42.485 1.000 21.62 HOH MOTA 2208 OW HOH 530 -4.689 10.177 46.511 1.000 31.65 ATOM 2209 OW HOH 531 1.545 35.657 50.866 1.000 19.59 MOTA 2210 OW HOH 532 0.980 22.687 36.818 1.000 30.57 ATOM 2211 OW HOH 533 -12.450 16.848 56.071 1.000 28.42 MOTA 2212 OW HOH 534 -9.418 16.139 51.364 1.000 22.60 ATOM 2213 OW HOH 535 32.711 25.816 43.116 1.000 31.44 2214 OW ATOM HOH 536 27.068 24.587 55.468 1.000 23.32 2215 OW ATOM HOH 537 13.523 11.832 51.199 1.000 10.73 2216 OW ATOM HOH 538 8.513 16.158 35.074 1.000 12.26 ATOM 2217 OW HOH 539 0.922 2.590 35.058 1.000 14.79 MOTA 2218 OW HOH 540 -1.548 34.484 1.000 14.25 MOTA 2219 OW HOH 541 11.711 16.898 30.416 1.000 17.84

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ATOM
       2220 OW
                 HOH
                     542 15.389
                                  11.536 32.065 1.000 17.88
       2221 OW
ATOM
                 HOH
                      543 18.496
                                          52.191 1.000 17.47
35.334 1.000 17.28
41.967 1.000 13.22
                                  6.995
       2222 OW
ATOM
                 HOH
                      544 19.848
                                  22.580
       2223 OW
ATOM
                 HOH
                      545 -0.387
                                  4.787
                                                  1.000 13.22
ATOM
       2224 OW
                                          35.308
33.926
                 HOH
                      546 23.502
                                  12.662
                                                  1.000 18.14
       2225 OW
ATOM
                 НОН
                      547 10.332
                                  25.236
                                                  1.000 19.05
ATOM
       2226 OW
                 нон
                      548 21.447
                                  20.605
                                                 1.000 17.24
                                          34.090
ATOM
       2227 OW
                 нон
                      549 8.164
                                          27.077 1.000 25.40
                                  7.685
ATOM
       2228 OW
                 HOH
                      550 14.393
                                  -5.127
                                          40.321 1.000 15.88
MOTA
       2229
            OW
                 НОН
                      551 12.873
                                  29.356
                                          39.662 1.000 16.45
ATOM
       2230 OW
                 HOH
                      552 11.974
                                  24.144
                                          58.426 1.000 19.71
ATOM
       2231 OW
                 HOH
                      553 17.521 7.949
                                          33.182 1.000 17.90
       2232
ATOM
            OW
                 НОН
                      554 3.401
                                  2.691
                                          43.340 1.000 23.76
MOTA
       2233 OW
                      555 18.669
                 HOH
                                          40.079 1.000 18.44
                                 28.057
       2234 OW
ATOM
                 HOH
                      556 10.827
                                          30.017 1.000 19.57
                                 12.928
       2235 OW
ATOM
                      557 20.630 16.270 66.466 1.000 20.84
                 HOH
       2236 OW
ATOM
                      558 11.315 20.266 64.044 1.000 21.62
                 HOH
       2237 OW
MOTA
                      559 26.277 14.516 43.946 1.000 16.22
                 HOH
       2238 OW
ATOM
                 HOH
                      560 9.616
                                  15.488 32.365 1.000 19.40
       2239 OW
ATOM
                 HOH
                      561 8.888
                                  4.903
                                          27.857 1.000 22.74
ATOM
       2240 OW
                      562 20.496
563 17.033
                 HOH
                                 -1.851 42.511 1.000 22.98
ATOM
       2241 OW
                 нон
                                 29.415 38.332 1.000 26.36
MOTA
       2242 OW
                 HOH
                      564 18.595
                                 6.141
                                          37.697 1.000 25.10
ATOM
       2243 OW
                      565 22.446
                                 13.893 31.420 1.000 29.00
                 HOH
ATOM
       2244 OW
                 HOH
                      566 6.586
                                  3.577
                                          28.350 1.000 27.82
MOTA
       2245 OW
                 HOH
                      567 6.250
                                  20.077
                                          30.961 1.000 23.27
ATOM
       2246 OW
                 HOH
                      568 7.341
                                  16.113
                                          31.186 1.000 28.59
MOTA
       2247 OW
                 HOH
                      569 16.090 32.070
                                          42.552
                                                 1.000 33.08
MOTA
       2248 OW
                                         37.258 1.000 25.17
58.591 1.000 28.58
                HOH
                      570 11.500
                                 28.806
       2249 OW
MOTA
                HOH
                      571 12.901
                                  26.768
       2250 OW
ATOM
                HOH
                      572 -17.071 17.043
                                          50.450
                                                  1.000 28.82
ATOM
       2251 OW
                HOH
                     573 25.262
                                          37.199 1.000 3.9.05
                                  7.705
       2252 OW
ATOM
                НОН
                     574 32.884
                                  26.440
                                         51.734 1.000 29.03
       2253 OW
ATOM
                HOH
                     575 -1.199
                                         42.527 1.000 14.86
                                 19.088
ATOM
       2254 OW
                HOH
                     576 -4.389
                                 33.026
                                          63.392 1.000 29.56
ATOM
       2255 OW
                     577 17.569 25.732
                HOH
                                          32.249 1.000 20.62
MOTA
       2256 OW
                HOH
                      578 -19.107 12.822
                                          67.516 1.000 22.35
ATOM
       2257 OW
                     579 29.333 19.198
                HOH
                                         51.975 1.000 22.51
       2258 OW
ATOM
                     580 27.950 27.635
                HOH
                                         51.903 1.000 25.40
       2259 OW
MOTA
                     581 -21.085 14.501
582 1.529 17.378
                HOH
                                         68.535 1.000 21.19
MOTA
       2260 OW
                HOH
                                         33.953 1.000 25.29
ATOM
       2261 OW
                     583 9.138 20.887 65.894 1.000 33.92
584 -11.896 19.091 44.780 1.000 17.48
                HOH
ATOM
       2262 OW
                HOH
ATOM
       2263 OW
                HOH
                     585 6.382
                                  12.597
                                         43.347 1.000 22.09
ATOM
       2264 OW
                HOH
                     586 17.762
                                  21.268
                                          29.046 1.000 20.79
ATOM
       2265 OW
                     587 -11.500 25.438
                HOH
                                         41.729 1.000 29.68
ATOM
       2266 OW
                нон
                     588 7.877
                                          29.689 1.000 27.70
                                  1.046
ATOM
       2267 OW
                     589 27.985
                НОН
                                  13.540 42.235 1.000 25.91
       2268 OW
ATOM
                     590 1.276
                HOH
                                  14.852
                                          34.021 1.000 20.41
MOTA
       2269 OW
                     591 24.622
                HOH
                                 24.179
                                          41.242 1.000 26.77
ATOM
       2270 OW
                нон
                     592 0.404
                                          36.006 1.000 27.92
57.827 1.000 31.86
                                  14.096
       2271 OW
MOTA
                HOH
                     593 -2.835
                                36.981
       2272 OW
ATOM
                     594 3.276
                HOH
                                  0.788
                                          39.940 1.000 32.07
       2273 OW
ATOM
                нон
                     595 11.025 -8.794
                                          31.468 1.000 27.18
       2274 OW
ATOM
                HOH
                     596 6.301
                                  2.276
                                          42.639
                                                 1.000 29.74
MOTA
       2275 OW
                HOH
                     597 29.302
                                         62.924 1.000 43.75
                                 16.146
ATOM
       2276 OW
                HOH
                     598 19.039
                                  20.964
                                          67.011
                                                  1.000 30.85
MOTA
       2277 OW
                HOH
                     599 8.380
                                  22.088
                                          64.518
                                                  1.000 42.62
ATOM
       2278 OW
                HOH
                     600 21.480
                                  10.826
                                          34.742
                                                  1.000 25.74
MOTA
       2279 OW
                HOH 601 -2.907
                                  21.956
                                         38.566
                                                  1.000 30.92
ATOM
       2280 OW
                НОН
                     602 -3.928
                                  29.841 43.352 1.000 43.96
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- 163 -ATOM 2281 OW нон 603 2.885 21.563 34.437 1.000 33.10 MOTA 2282 OW HOH 604 11.801 6.043 25.270 1.000 38.18 ATOM 2283 OW HOH 605 -1.019 17.197 40.472 1.000 18.48 ATOM 2284 OW HOH 606 18.382 23.349 68.110 1.000 22.54 ATOM 2285 OW HOH 607 -8.141 8.137 45.609 1.000 17.64 ATOM 2286 OW HOH 608 5.022 2.667 51.700 1.000 24.29 ATOM 2287 OW HOH 509 17.557 10.755 33.490 1.000 21.94 ATOM 2288 OW НОН 610 11.222 1.201 49.675 1.000 20.61 ATOM 2289 OW HOH 611 4.243 35.047 50.509 1.000 22.18 ATOM 2290 OW HOH 612 11.103 4.031 56.082 1.000 22.08 ATOM 2291 OW HOH 613 11.366 31.522 36.791 1.000 32.32 2292 OW MOTA HOH 614 -21.189 24.787 52.739 1.000 31.83 2293 OW ATOM 615 7.847 HOH -1.491 30.674 1.000 24.77 ATOM 2294 OW 616 19.041 HOH 11.937 31.445 1.000 25.97 ATOM 2295 OW HOH 617 6.221 29.879 40.410 1.000 29.24 MOTA 2296 OW HOH 618 17.266 5.933 35.280 1.000 23.72 2297 OW ATOM HOH 619 5.983 -7.215 28.510 1.000 28.19 2298 OW ATOM НОН 620 22.574 8.129 57.639 1.000 30.97 2299 OW ATOM HOH 621 2.553 7.806 60.287 1.000 28.77 ATOM 2300 OW HOH 622 29.939 25.812 51.234 1.000 34.00 ATOM 2301 OW нон 623 2.205 34.823 53.632 1.000 25.88 ATOM 2302 OW HOH 624 18.091 13.838 67.343 1.000 28.46 ATOM 2303 OW HOH 625 8.342 58.475 1.000 26.84 3.195 ATOM 2304 OW 42.790 1.000 31.11 35.620 1.000 27.48 42.834 1.000 32.55 HOH 626 -16.086 18.427 ATOM 2305 OW HOH 627 -2.098 13.445 ATOM 2306 OW 628 0.481 HOH 30.471 ATOM 2307 OW 629 13.368 HOH 42.899 1.000 28.70 33.845 ATOM 2308 OW HOH 630 -13.792 14.642 51.533 1.000 25.58 2309 OW MOTA HOH 631~3.299 29.242 1.000 39.62 1.461 MOTA 2310 OW 1.000 27.75 HOH 632 -16.012 20.690 46.705 ATOM 2311 OW нон 633 19.606 8.142 31.259 1.000 27.02 ATOM 2312 OW HOH 634 5.077 7.954 57.205 1.000 30.59 ATOM 2313 OW HOH 635 -1.502 6.963 45.877 1.000 35.68 ATOM 2314 OW нон 636 9.974 38.804 1.000 21.84 17.449 ATOM 2315 OW нон 637 -22.829 12.836 67.228 1.000 25.04 2316 OW ATOM НОН 638 6.275 34.333 39.722 1.000 25.88 ATOM 2317 OW HOH 639 2.248 56.051 1.000 26.67 19.798 MOTA 2318 OW HOH 640 -20.552 17.013 67.454 1.000 31.34 ATOM 2319 OW HOH 641 9.298 16.570 28.911 1.000 29.96 ATOM 2320 OW HOH 642 - 1.73211.113 60.074 1.000 28.13 ATOM 2321 OW НОН 643 34.157 23.604 44.657 1.000 36.36 ATOM 2322 OW HOH 644 24.298 20.199 33.576 1.000 34.90 ATOM 2323 OW нон 645 13.803 -4.667 1.000 32.66 31.570 MOTA 2324 OW HOH 646 6.295 -2.594 1.000 34.61 29.009 MOTA 2325 OW нон 647 5.623 37.039 49.318 1.000 28.08 MOTA 2326 OW HOH 648 -18.805 19.286 46.868 1.000 38.32 2327 OW ATOM нон 649 16.026 35.829 49.382 1.000 34.45 ATOM 2328 OW HOH 650 -12.187 28.769 45.330 1.000 27.36 ATOM 2329 OW HOH 651 21.344 5.778 55.101 1.000 27.43 MOTA 2330 OW 652 -1.848 нон 2.125 32.240 1.000 32.02 ATOM 2331 OW нон 653 -14.568 18.811 55.775 1.000 29.95 ATOM 2332 OW HOH 654 -8.655 26.254 38.301 1.000 32.07 ATOM 2333 OW нон 655 18.836 13.542 28.102 1.000 32.24 ATOM 2334 OW HOH 656 16.217 14.669 25.619 1.000 33.35 ATOM 2335 OW HOH 657 28.678 14.477 38.043 1.000 30.94 ATOM 2336 OW 658 -11.834 15.408 нон 53.330 1.000 33.25 ATOM 2337 OW 659 -1.317 HOH 38.273 59.599 1.000 34.45 ATOM 2338 OW HOH 660 8.784 13.918 28.681 1.000 33.62 ATOM 2339 OW HOH 661 -3.058 14.508 47.405 1.000 28.79 ATOM 2340 OW НОН 662 10.968 33.651 38.533 1.000 36.21 MOTA 2341 OW НОН 663 28.960 21.602 53.665 1.000 29.25

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CLAIMS

- Deacetoxycephalosporin C synthase (DAOCS) having a structure designated by the X-ray co-ordinates of structure A or structure B herein.
- 2. DAOCS in the form of a complex with a metal, e.g. iron or lead, and optionally in the presence of a substrate and/or a substrate analogue or inhibitor, having a structure designated by the X-ray co-ordinates herein.
- 3. DAOCS as claimed in claim 2, wherein the substrate is penicillin N, penicillin G, 2-oxoglutarate or dioxygen, and the inhibitor is selected from N-oxalylamino acids, pyridine-carboxylates and nitrous oxide.
- 4. Use of the three-dimensional structure of DAOCS for the modification of DAOCS or other related 2-oxoglutarate dependent enzyme.
 - 5. Use as claimed in claim 4, wherein the related 2-oxoglutarate dependent enzyme is DACS, DAOC/DACS or the oxygenase enzyme involved in the introduction of the 7α -methoxy group into cephamycin C.
 - 6. Use as claimed in claim 5 for the modification of DAOCS, DACS or DAOC/DACS such that they accept unnatural substrates more efficiently than the wild type enzymes.

7. Use as claimed in claim 5 for the modification of DAOCS, DACS, DAOC/DACS such that they convert natural substrates to pharmaceuticals or useful intermediates in the preparation of pharmaceuticals.

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8. Use as claimed in claim 6 wherein the unnatural substrates are penicillins including penicillin G, penicillin V, 6-aminopenicillanic acid, amoxycillin, or penicillins with a phenyl glycine or p-hydroxyphenyl glycine side chain.

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- 9. Use as claimed in claim 6 wherein the unnatural substrate is a cephalosporin.
- 10. Use as claimed in claim 6 wherein the unnatural substrate is an amino acid, including the proteinogenic amino acids, or a peptide.
 - 11. Use as claimed in any one of claims 6-8, wherein penicillin G, penicillin V, another unnatural substrate or penicillin N is converted to a cephalosporin or exomethylene cephalosporin.

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An enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the side chain binding site of penicillin N or DAOC is modified and at at least one of the following sites at least one amino acid residue is changed to another amino acid residue or is deleted: Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

An enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the penicillin/cephalosporin binding site of penicillin N or DAOC is modified and at at least one of the following amino acid residues is changed or deleted: Ile88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Ile305, Arg306, Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

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- 14. An enzyme according to claim 12 or claim 13 which is a mutant of DAOCS or DACS or DAOC/DACS.
- 15. An enzyme as claimed in any one of claims 12-14, wherein both the side chain and the penicillin/cephalosporin binding sites of penicillin N or DAOC are modified and at least one of the residues specified in claims 12 and 13 is changed or deleted.
 - 16. An enzyme as claimed in any one of claims 12-15, wherein
 two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.
 - 17. A gene encoding for the enzyme of any one of claims 12-16.

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- 18. A micro-organism capable of expressing the gene of claim 17 under fermentation conditions.
- 19. Use of micro-organisms of claim 18 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

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- 20. Use as claimed in claim 19 wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway including isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 21. A method which comprises using the three-dimensional structure of DAOCS for determining or predicting the structure of another related 2-oxoglutarate dependent enzyme or related enzyme not from the penicillin and cephalosporin biosynthesis pathway, and using the structural information so obtained for modifying the other enzyme or for designing an inhibitor for the other enzyme.
- 22. A method as claimed in claim 21 wherein the said other
 related 2-oxoglutarate dependent enzyme or related enzyme is
 1-aminocylopropane-1-carboxylate oxidase, gibberellin C-20 oxidase, flavone synthase, flavanone 3β-hydroxylase, hyoscyamine 6β-hydroxylase, prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, lysyl hydroxylase, proline hydroxylases, γ-butyrobetaine hydroxylase, enzymes
 in herbicide resistance mechanisms, clavaminate synthase, an oxygenase enzyme involved in the biosynthesis of carbapenems, the so called ethylene forming enzyme from *Pseudomonas syringe*, p-hydroxyphenylpyruvate dioxygenase, and an oxygenase enzyme involved in the oxidation of phytol in human liver peroxisomes.

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A method as claimed in claim 21 or 22, wherein the said other enzyme is modified, by deletion or addition or alteration; at one or more of the sites defined in claim 12 or claim 13; or using the following information for the design or an inhibitor: Asp185, His183 and His243 act as ligands to the iron; Arg258 and Ser260 and the Fe bind the

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2-oxoglutarate; Met180, Phe225, Leu31 and Val245 are close to the iron binding site; Tyr33, Arg160, Arg162, Phe164, Ile192, Gln194, Leu204, Leu223, Leu215 are important for the construction of the part of the active site binding 2-oxoglutarate; and Arg160 and Arg162 are important for binding an amino acid or peptide derived substrate.

- A method as claimed in any one of claims 21-23, wherein the said other enzyme is prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, or lysyl hydroxylase and the inhibitor is to be used for the treatment of human diseases including fibrotic diseases including liver cirrhosis and arthritis.
- 25. A method as claimed in any one of claims 21-23, wherein the said other enzyme is p-hydroxyphenylpyruvate dioxygenase and the inhibitor is to be used in the treatment of certain genetic disorders.
- 26. A method as claimed in any one of claims 21-23, wherein the said other enzyme is involved in herbicide resistance and the information is to be used to design new herbicides to overcome the problem of resistance.

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INTERNATIONAL SEARCH REPORT

Inte. Jonal Application No PCT/GB 98/03860

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A. CLASS IPC 6	SIFICATION OF SUBJECT MATTER C12N15/52 C12N9/00 C12P35	5/00		- 4.
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X Further	er documents are listed in the continuation of box C.	X Patent family memb	bers are listed i	n annex.
° Special cate	egories of cited documents :	"T" later decument published		
"A" documer	nt defining the general state of the art which is not ered to be of particular relevance	"T" later document published or priority date and not cited to understand the	in conflict with t	the application but
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Date of the ad	ctual completion of the international search	Date of mailing of the in	ternational sear	rch report
	March 1999	26/03/1999	1	
Name and ma	ailing address of the ISA European Patent Office, P.B. 5818 Patentlaan 2	Authorized officer		
	NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nł.			
	Fax: (+31-70) 340-3016	Hix, R		

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